Barcelona Supercomputing Center
Centro Nacional de Supercomputación

UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH

Modeling dust mineralogy and its impacts on the Earth System

María Gonçalves Ageitos

Associated researcher

Atmospheric Composition Group. Earth Sciences Department. BSC.

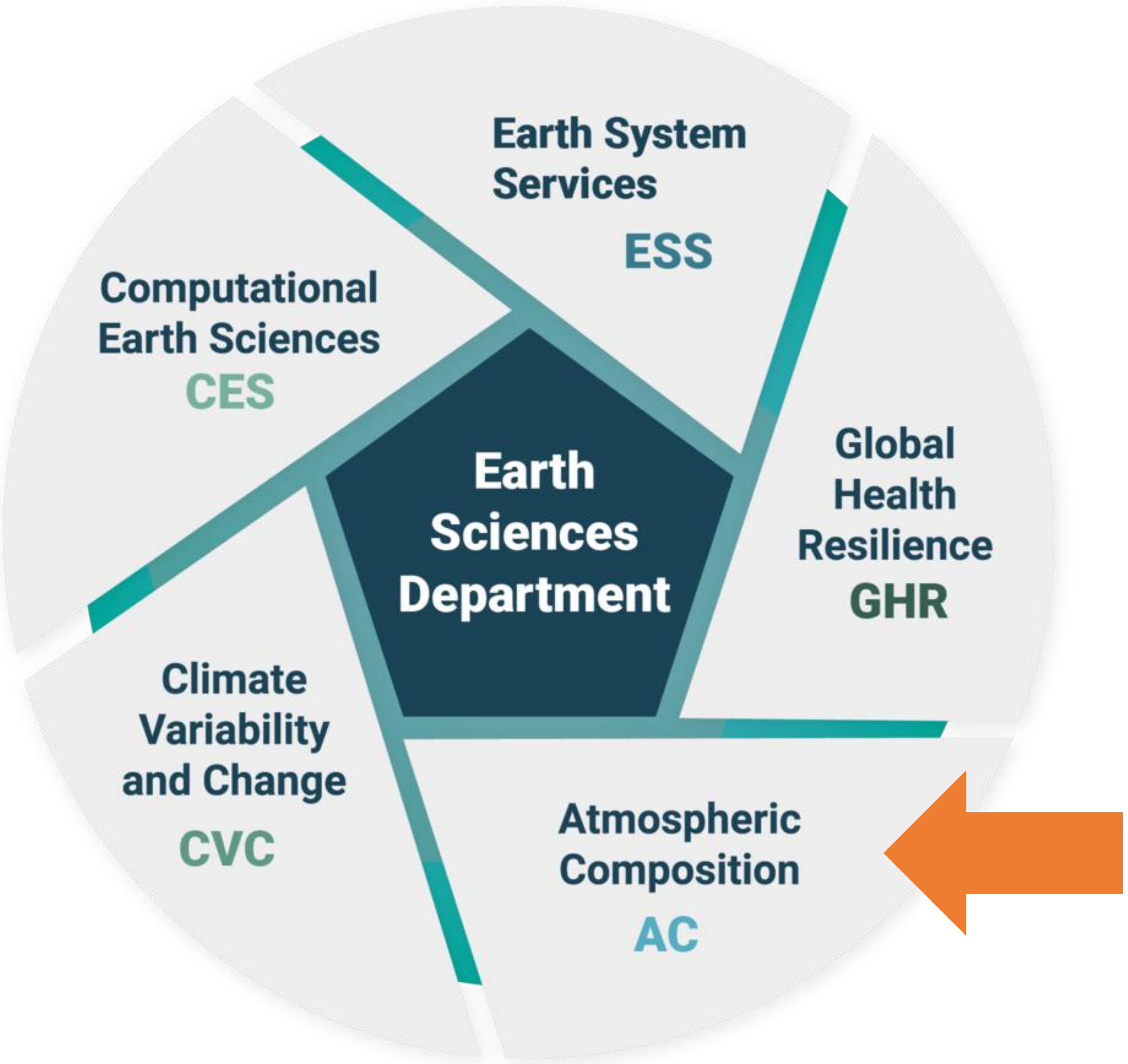
Associated professor

Project and Construction Engineering Department. UPC.

GFDL seminar

Princeton, NJ. 06/06/2023

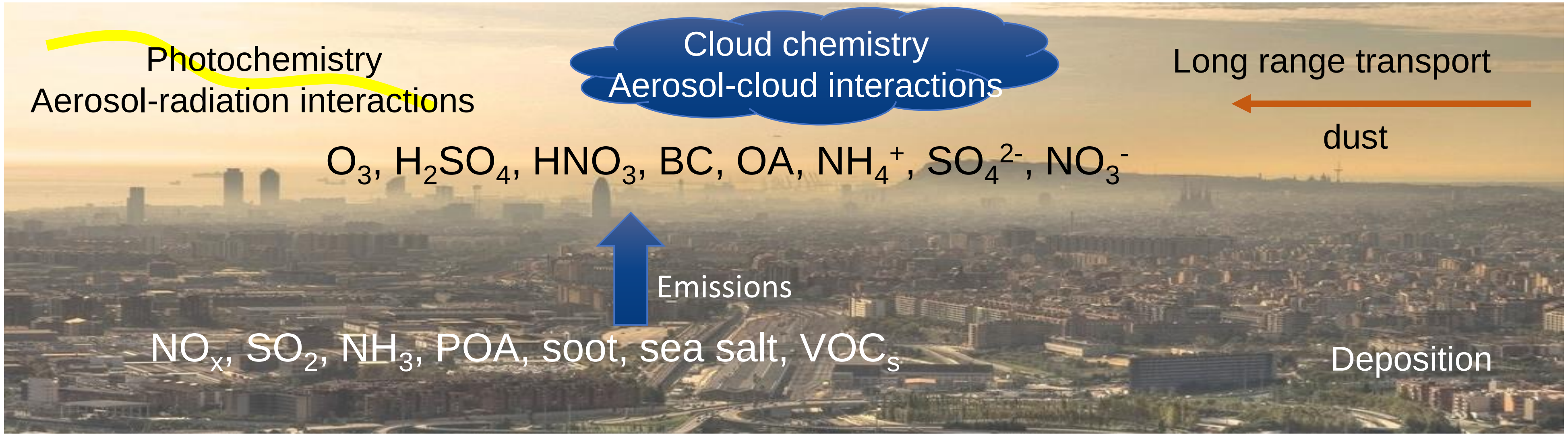
The Earth Sciences Department at BSC



Carlos Pérez García-Pando (carlos.perez@bsc.es)
Oriol Jorba (oriol.jorba@bsc.es)
20 people

AC Main goal

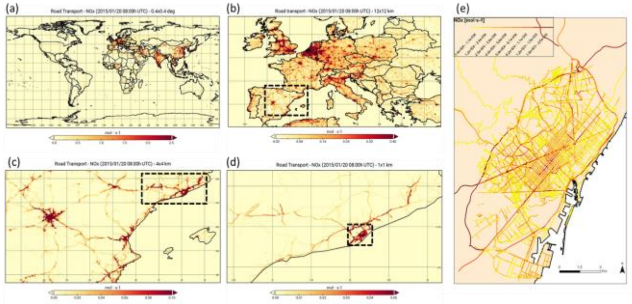
To understand, constrain and predict the spatiotemporal variations of atmospheric pollutants across scales along with their effects upon air quality, health, weather and climate.



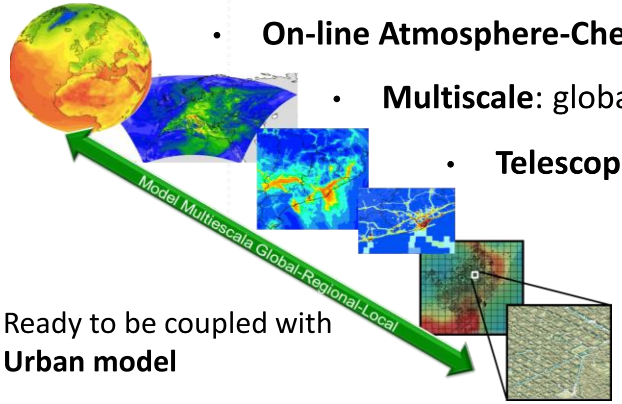
Model and tool developments

HERMESv3

A **python-based, open source, parallel and multiscale** emission model



MONARCH

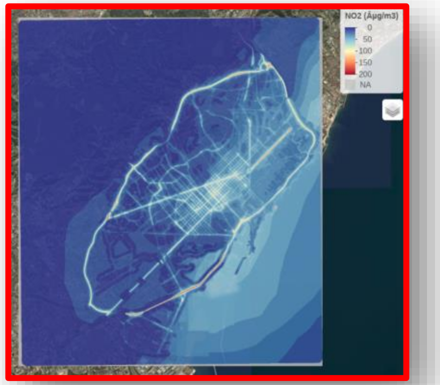


- **On-line Atmosphere-Chemistry coupling**
- **Multiscale**: global to local (1km)
- **Telescoping nesting**

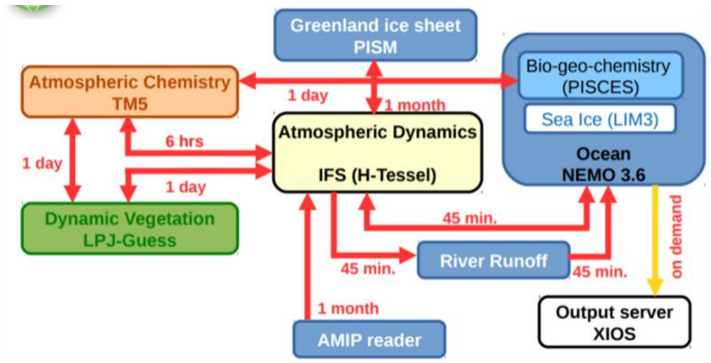
Ready to be coupled with **Urban model**

CALIOPE-Urban

Street-scale dispersion model



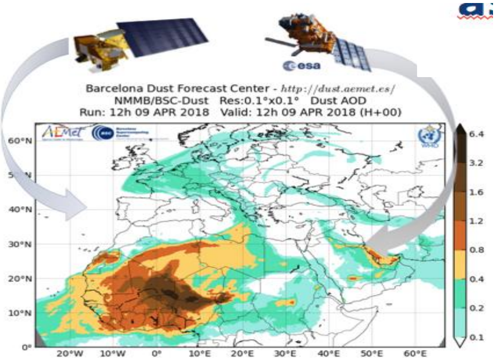
EC-Earth3-AerChem



Schematics of the EC-Earth version 3 components and the coupling frequency between them.

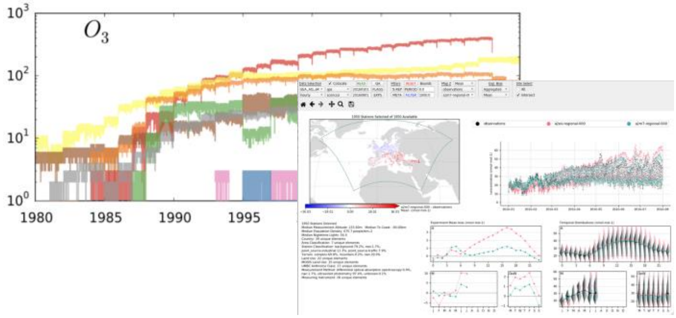
LETKF DA

Ensemble based Data Assimilation system



GHOST/Providentia

Harmonised treatment of observations and **dynamic/flexible evaluation** system

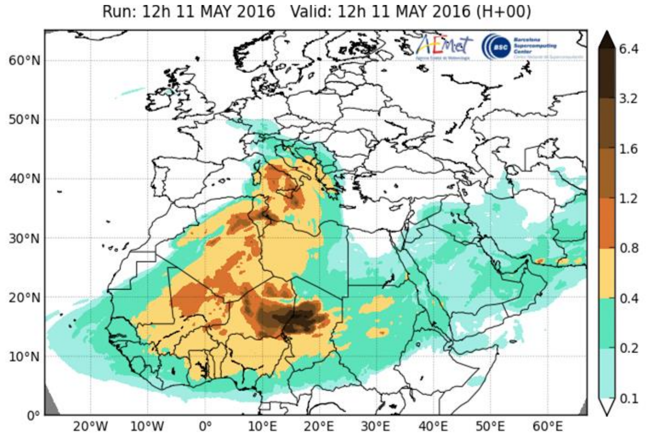


In collaboration with CES, ESS and CVC

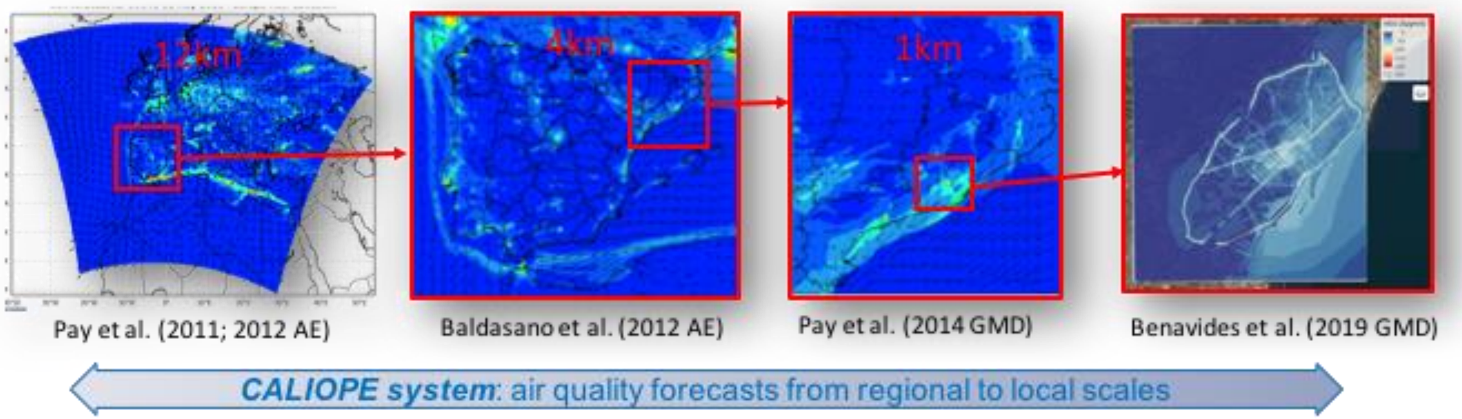
Forecasts, reanalysis, services

WMO Dust Regional Centers

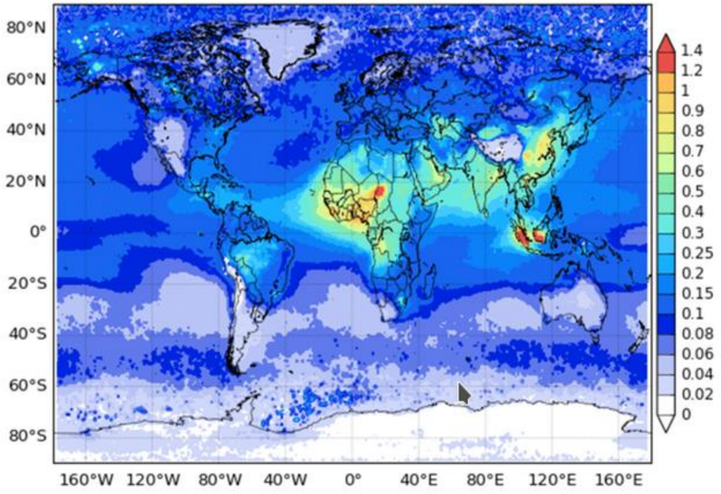
Dust forecasts and and renalysis



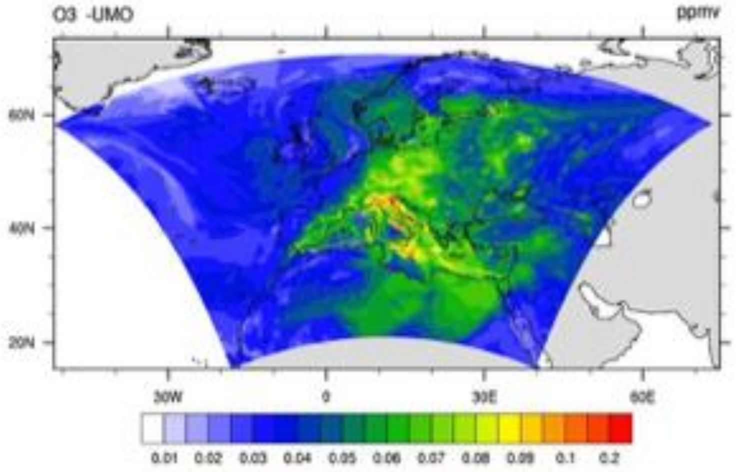
CALIOPE Air Quality Forecast system



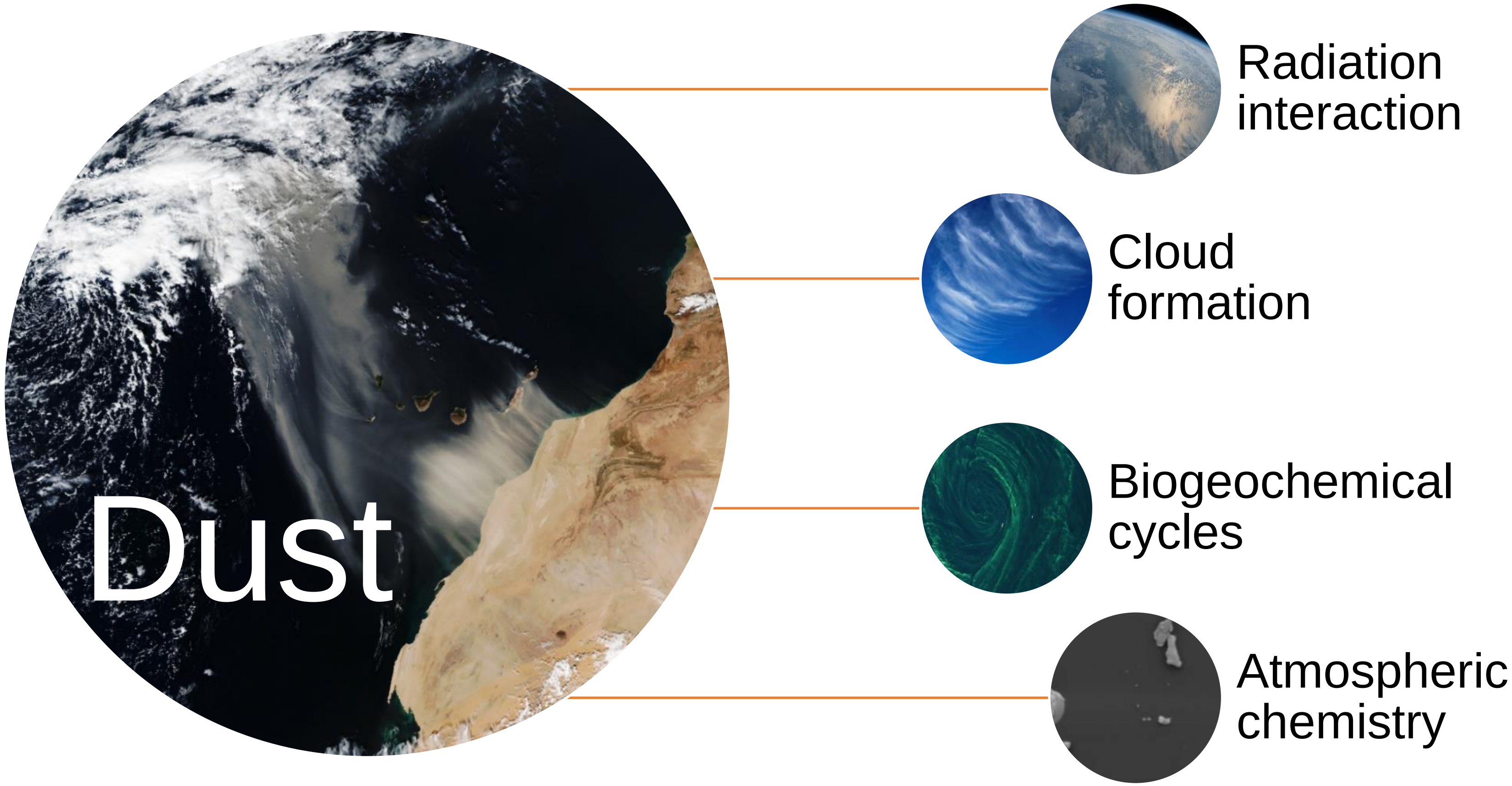
ICAP global aerosol ensemble



CAMS air quality regional ensemble



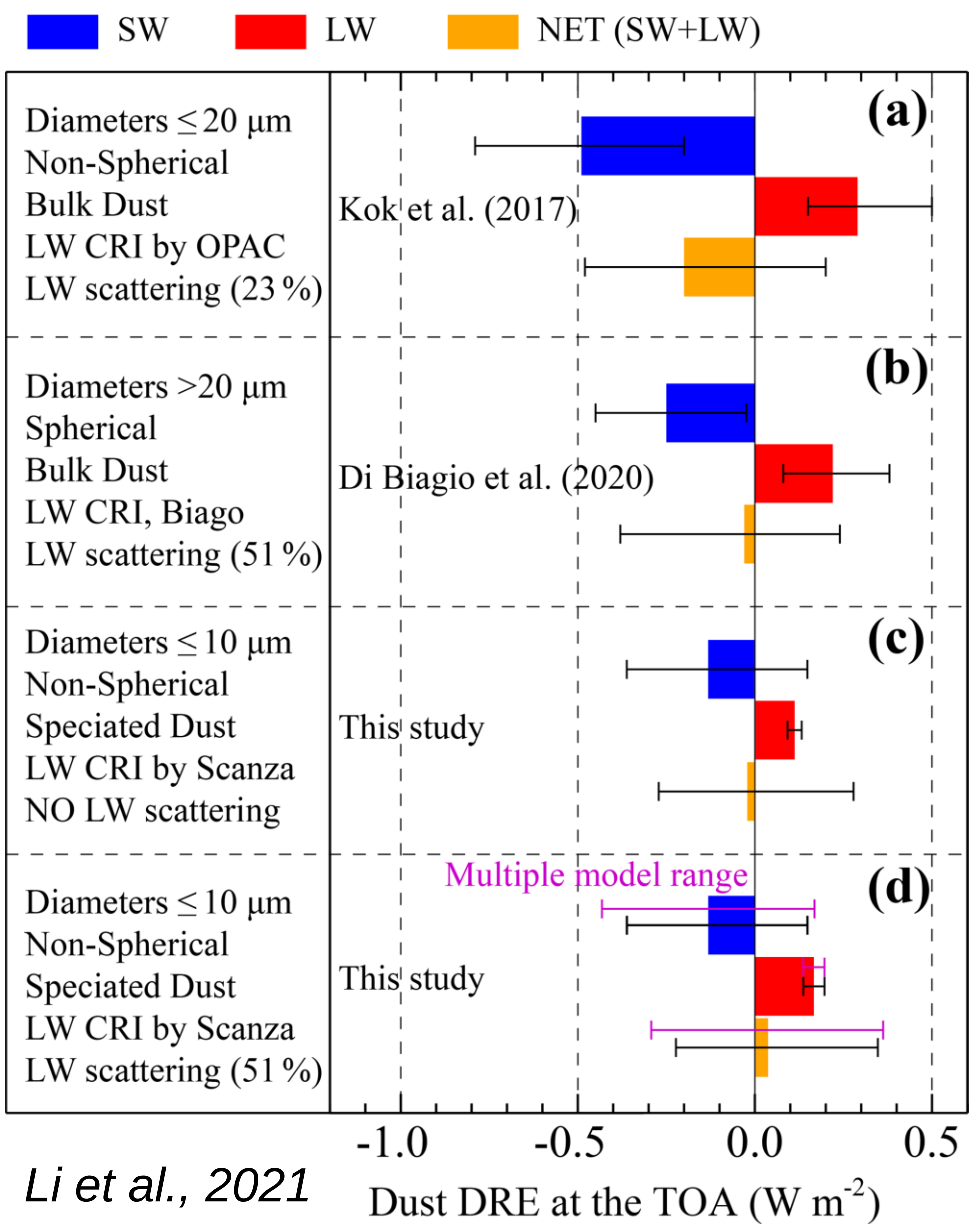
Dust mineralogy modeling



… these impacts are modulated by mineralogy.

Image credits: NASA, NOAA, Krueger et al. (2004)

Dust interaction with radiation



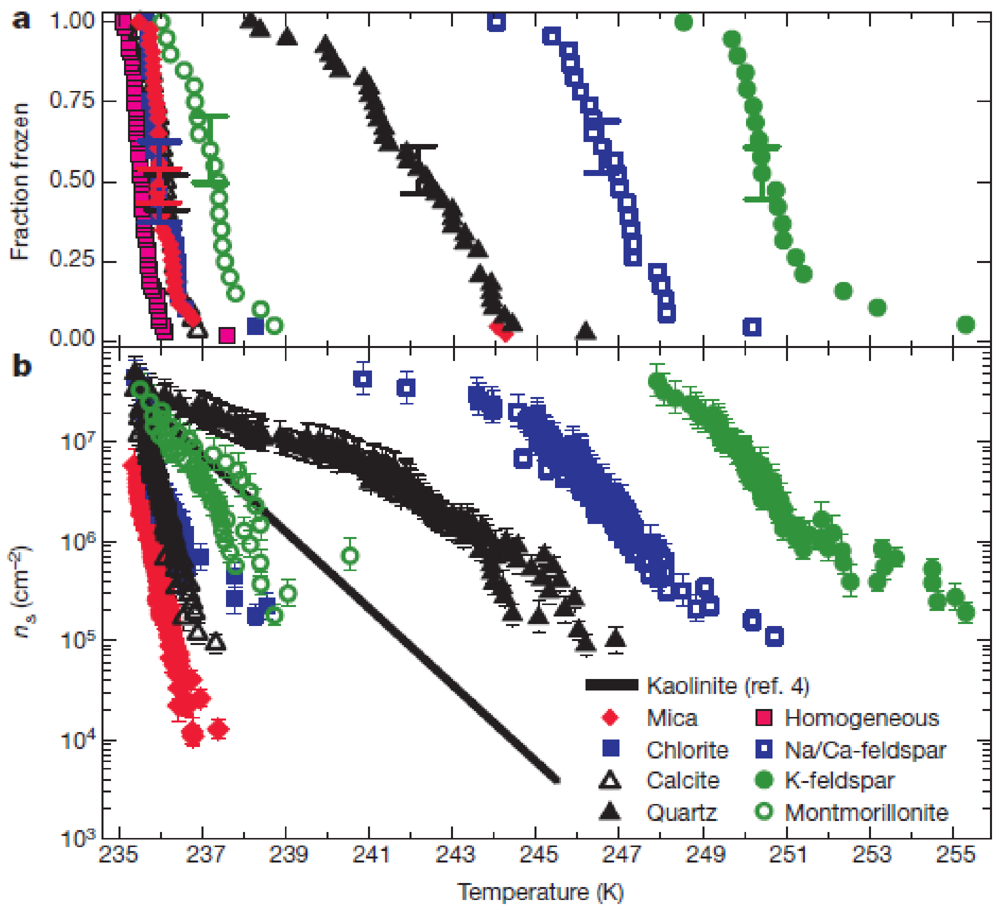
Li et al., 2021

- **Dust absorption** in the **shortwave** linearly correlates with the amount of **iron oxides** (e.g., DiBiagio et al., 2019; Möosmuller et al., 2012)

- Li et al. (2021) multi-model study **attributes 97% of the uncertainty range** in **dust DRE** to uncertainties in the abundance of **iron oxides**.

Dust as ice nuclei

- **K-feldspars** (Atkinson et al., 2013), and **quartz** (Harrison et al., 2019) have been singled out as **effective ice nuclei**.

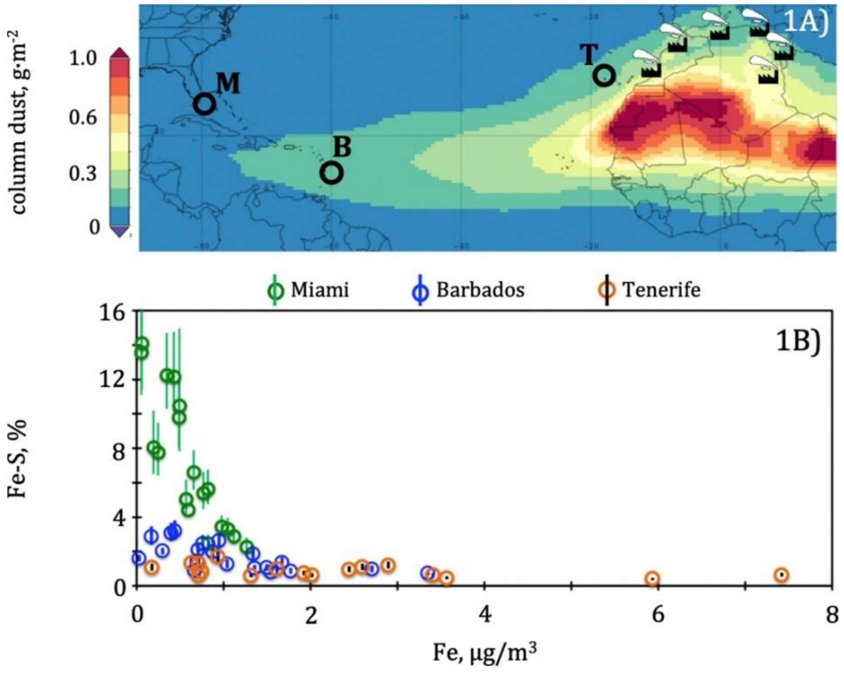


Experimental results showing k-feldspar particles freezing at warmer temperatures than other mineral components

Fraction of droplets (top) and nucleation site density (bottom), with 14–16 µm in diameter and containing a range of minerals in dust, frozen as a function of temperature during cooling, as detected in Atkinson et al. 2013 experiments.

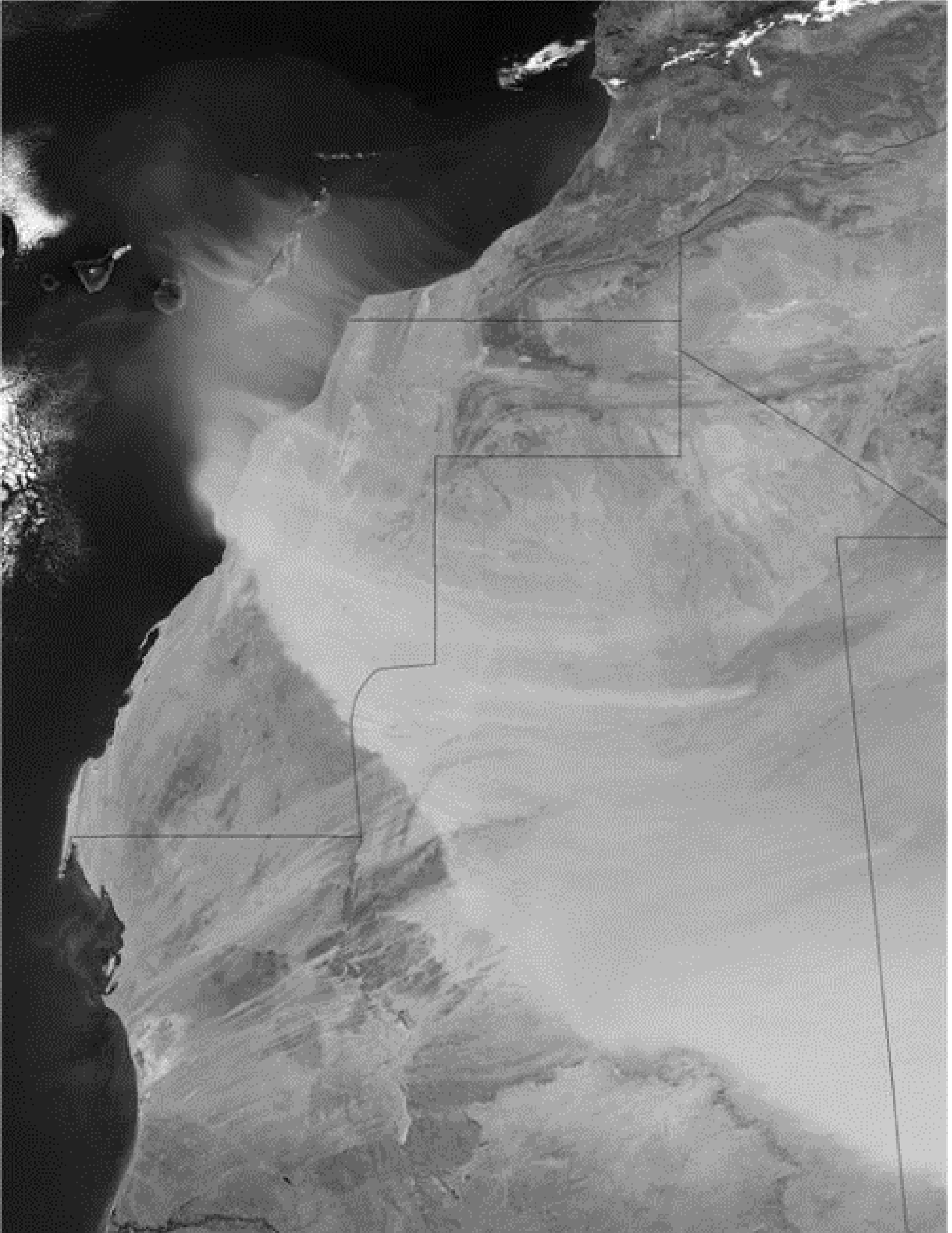
Nutrients in dust

- Mineral dust is a relevant source of **dissolved iron** to open ocean waters (e.g. Jickells et al., 2005; Conway et al. 2014), and it has been found to play a role on the fertilization of the Amazon forest (e.g. Yu et al., 2015).
- The **iron content**, but also its **solubility** is related to the dust mineral composition (e.g. Journet et al., 2009, Shi et al., 2011; Shi et al., 2012).



Rodriguez et al. (2021)

Iron solubility (Fe–S) versus iron in samples collected in Tenerife, Barbados and Miami during July and August 2015.



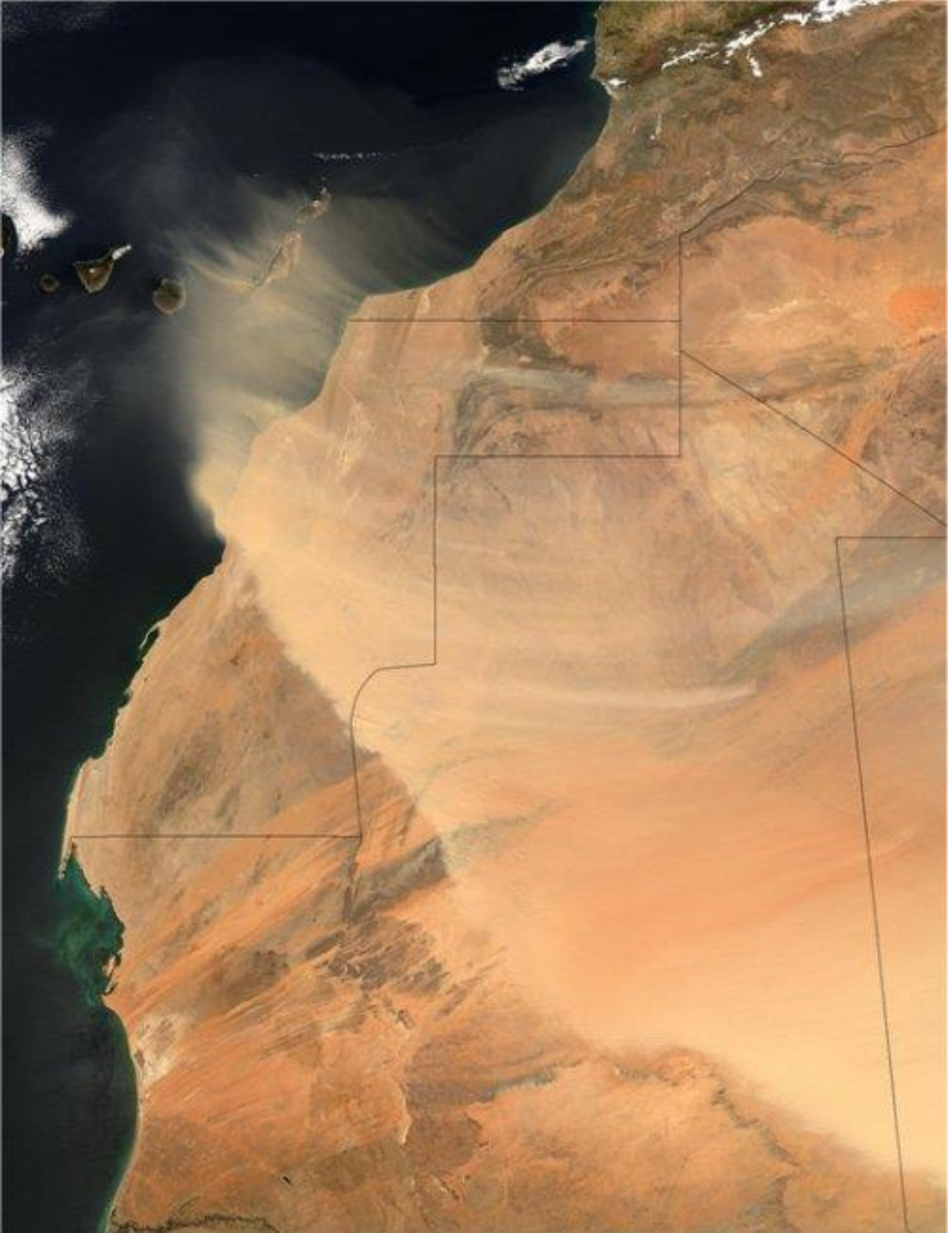
Credit: NASA - The Visible Earth. Jacques Descloitres, MODIS Rapid Response Team, NASA/GSFC

Many ESMs still consider dust as a homogeneous species, mainly because of…

… our limited knowledge of the composition of parent soils

… and the resulting size-distributed mineralogy at emission,

… and, to a lesser extent, the increase in computational burden.



Many ESMs still consider dust as a homogeneous species, mainly because of…

… our limited knowledge of the composition of parent soils

… and the resulting size-distributed mineralogy at emission,

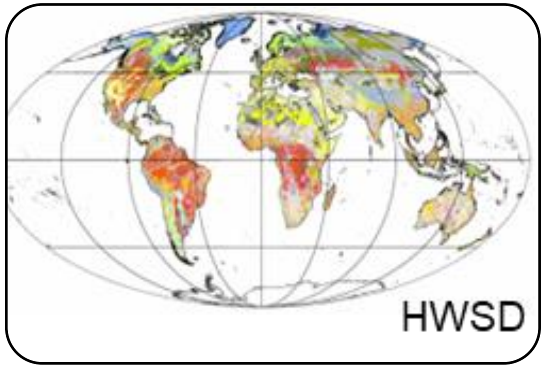
… and, to a lesser extent, the increase in computational burden.

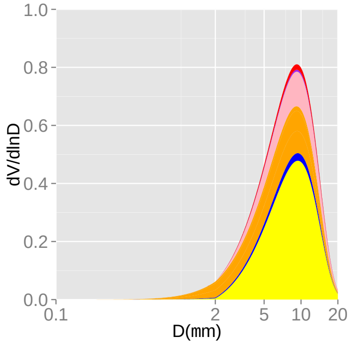
Credit: NASA - The Visible Earth.
Jacques Descloitres, MODIS Rapid Response Team, NASA/GSFC

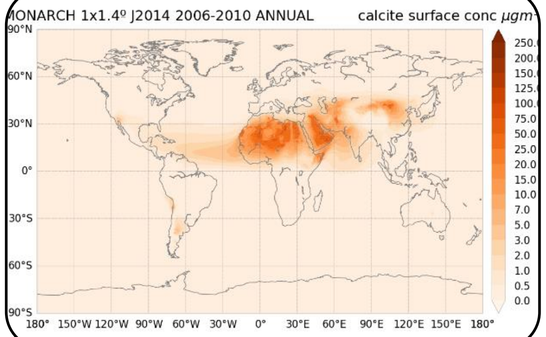
Today:

- Our current understanding of the airborne dust mineralogy
- Impact of considering mineralogy in different aspects of the climate system
- Open questions and future research

Modelling dust mineralogy







Soil mineralogy

Emitted size-resolved mineral fractions

Minerals' atmospheric cycle

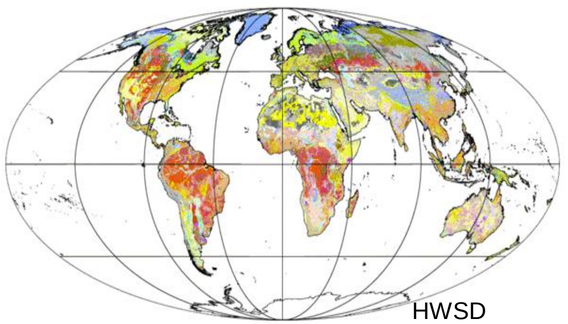
Global soil mineralogy atlases

- **Claquin et al. 1999, Nickovic et al. 2012**: 8 minerals. *C1999*

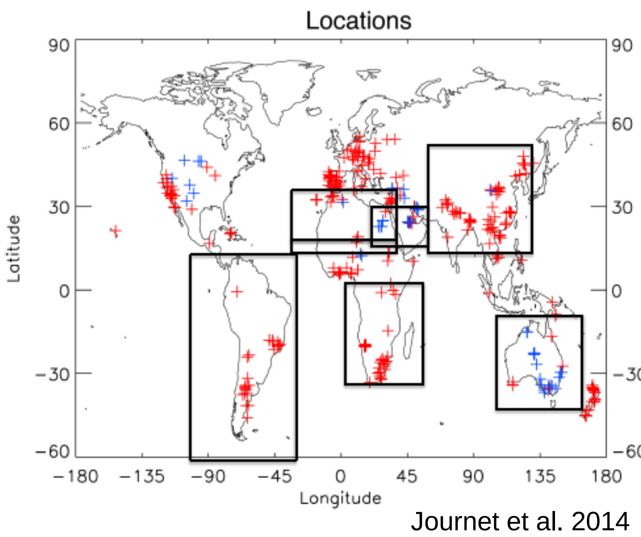
Illite, smectite, kaolinite, quartz, feldspars, calcite, gypsum and hematite (iron oxides).

- **Journet et al. 2014**: 12 minerals. *J2014*

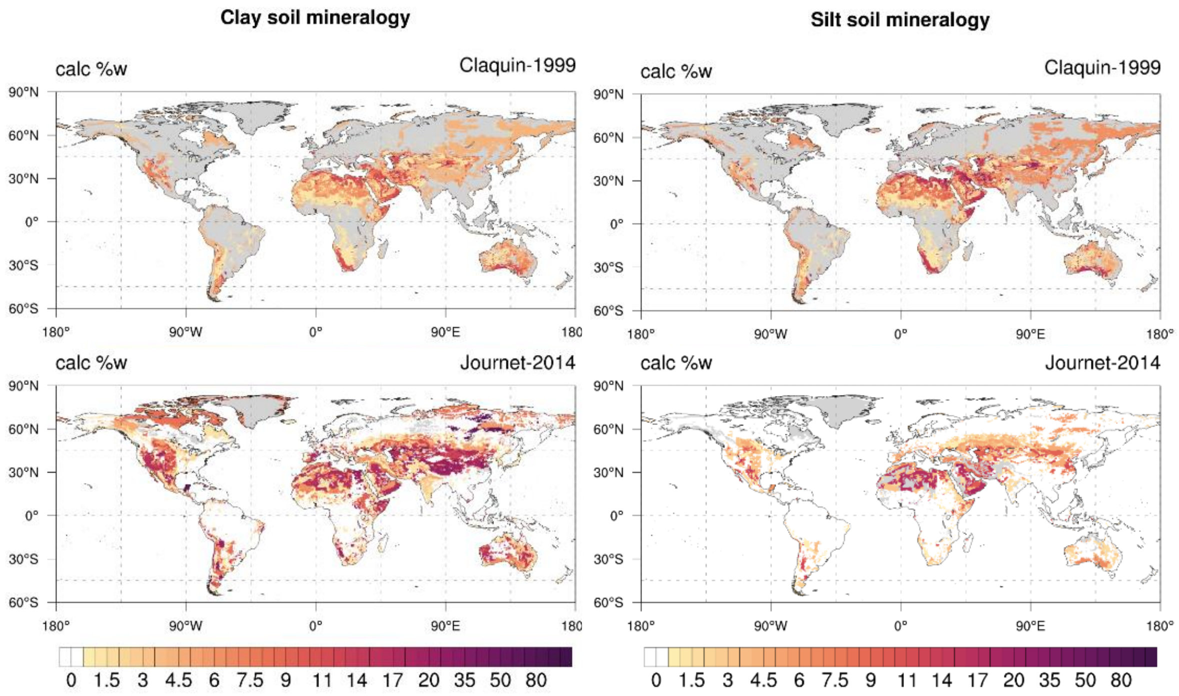
Illite, smectite, kaolinite, vermiculite, chlorite, mica, quartz, feldspars, calcite, gypsum, hematite and goethite.



FAO soil classification



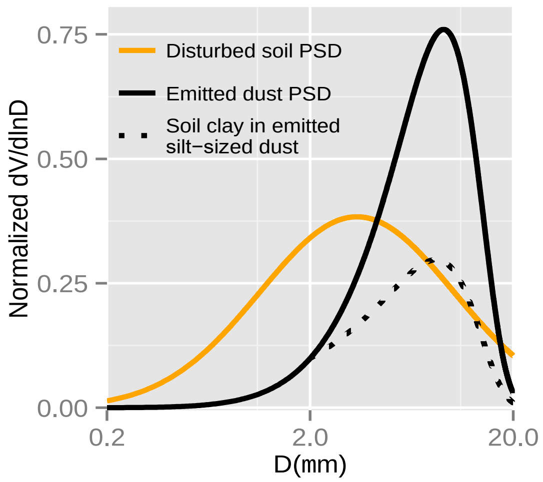
Mean mineralogy

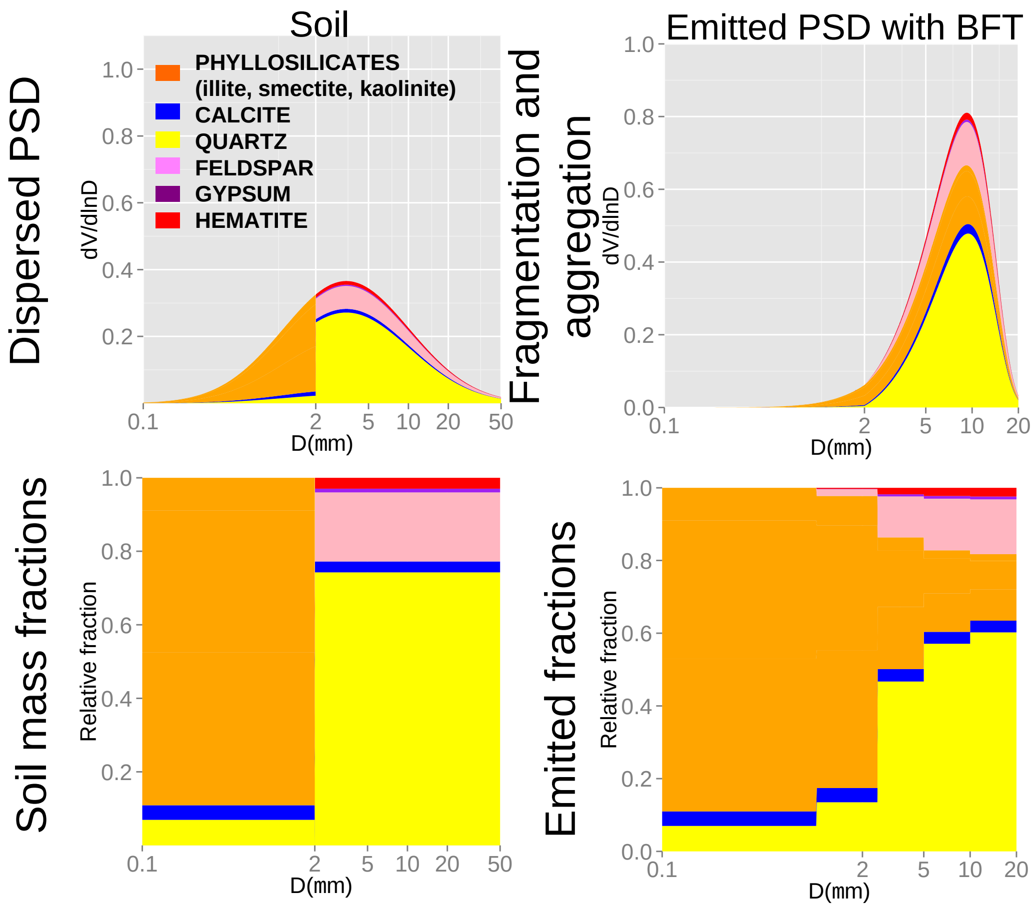


Mineralogical composition for clay (ϕ < 2 µm) and silt (ϕ 2-63 µm) size classes

Dust emitted PSD and mineralogy

Brittle Fragmentation Theory
(Kok, 2011)



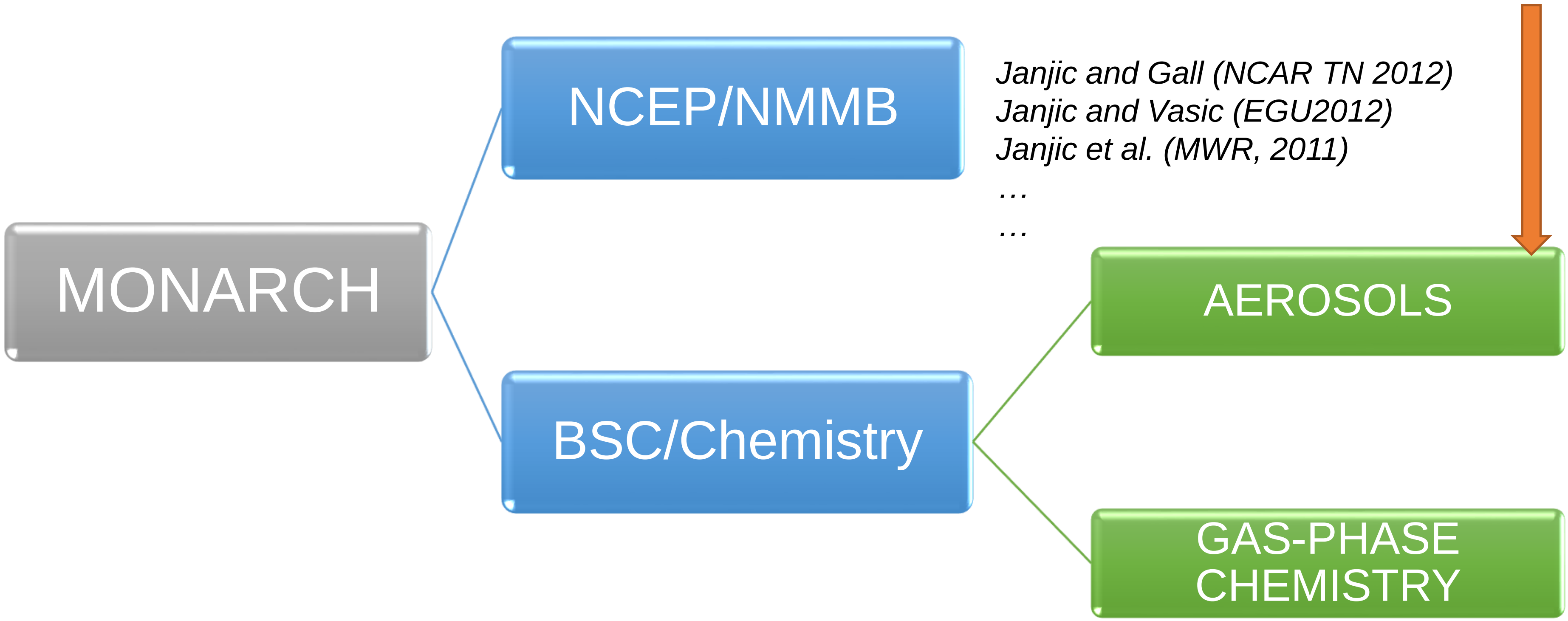


Perlwitz et al., 2015a,b;
Pérez García-Pando et al., 2016;
Pérez García-Pando et al., in prep

The MONARCH model

- ***Multiscale***: global to regional (up to 1km) scales allowed
- Fully ***on-line*** coupling: weather-chemistry feedback processes allowed
- Enhancement with a ***data assimilation*** system

Dust mineralogy

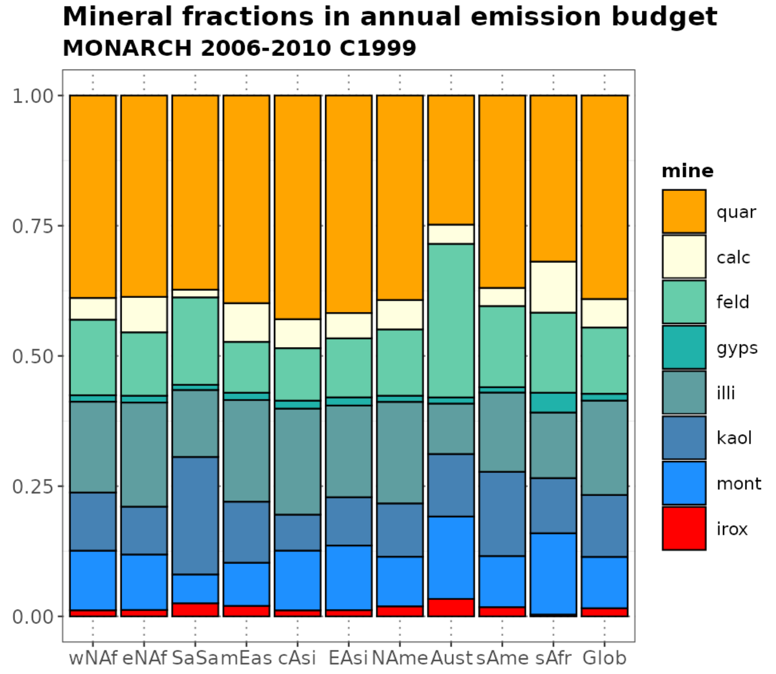


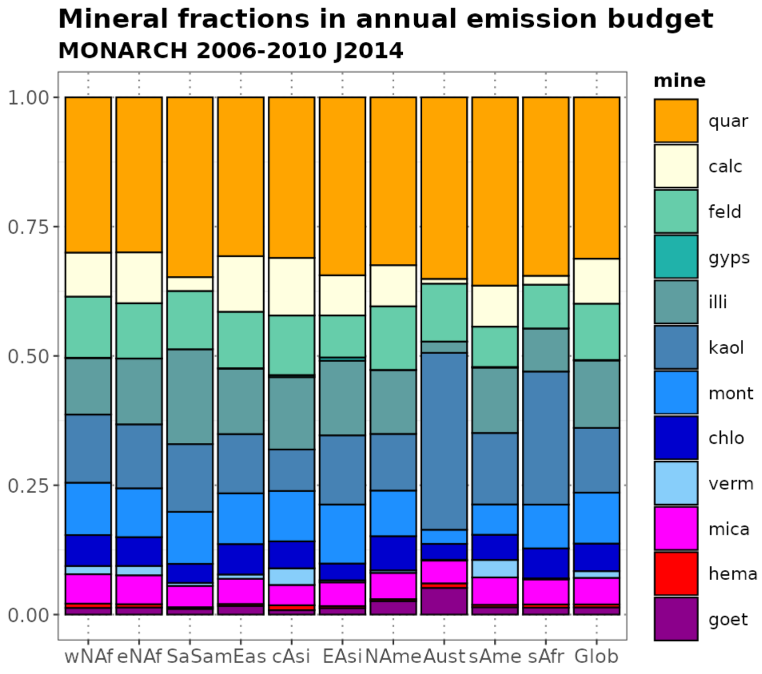
Janjic and Gall (NCAR TN 2012)
Janjic and Vasic (EGU2012)
Janjic et al. (MWR, 2011)
…
…

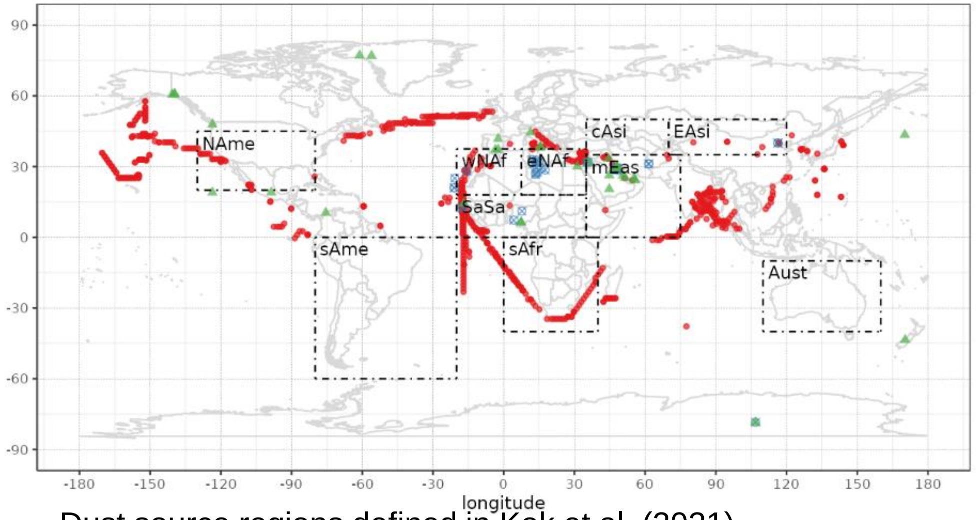
Pérez et al. (ACP, 2011)
Haustein et al. (ACP, 2012)
Spada et al. (ACP, 2013)
Spada et al. (AE, 2014)
Spada (2015)
Di Tomaso et al. (GMD, 2017)
Klose et al. (ACP, 2021)
Gonçalves Ageitos et al. (ACP, in review)
Ilic et al. (in prep)

Jorba et al. (JGR, 2012)
Badia and Jorba (AE, 2014)
Badia et al. (GMD; 2017)

Emitted dust mineralogy according to MONARCH C1999 and J2014







Dust source regions defined in Kok et al. (2021)

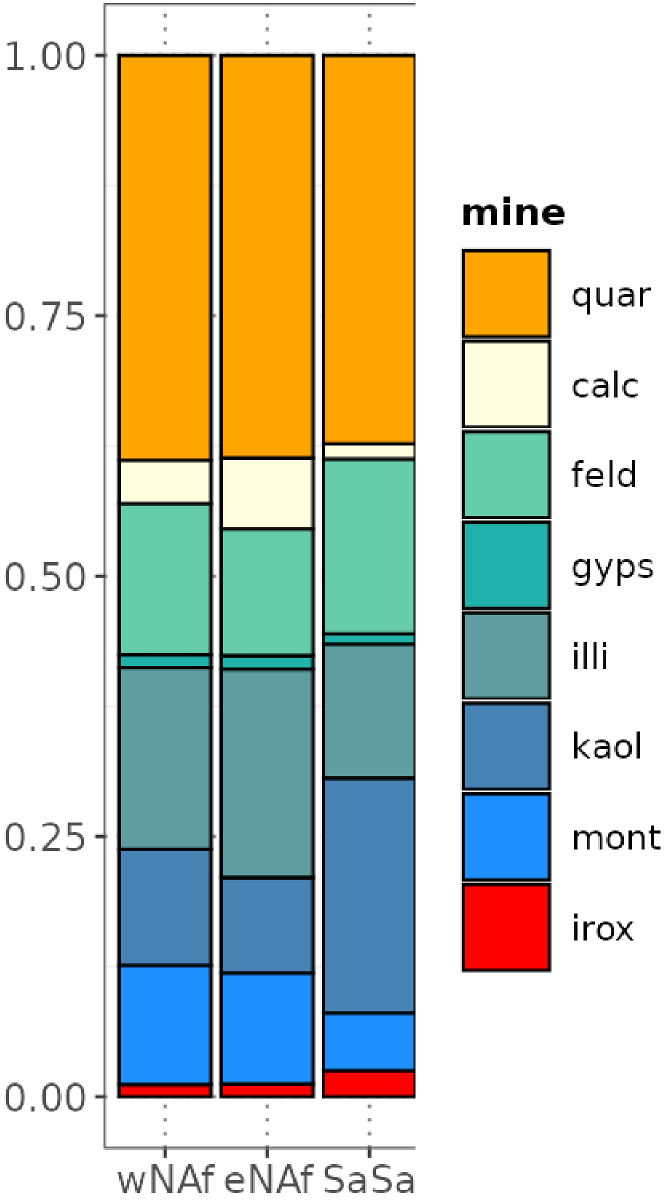
Emitted mass fractions per region and globally depending on the soil map used

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

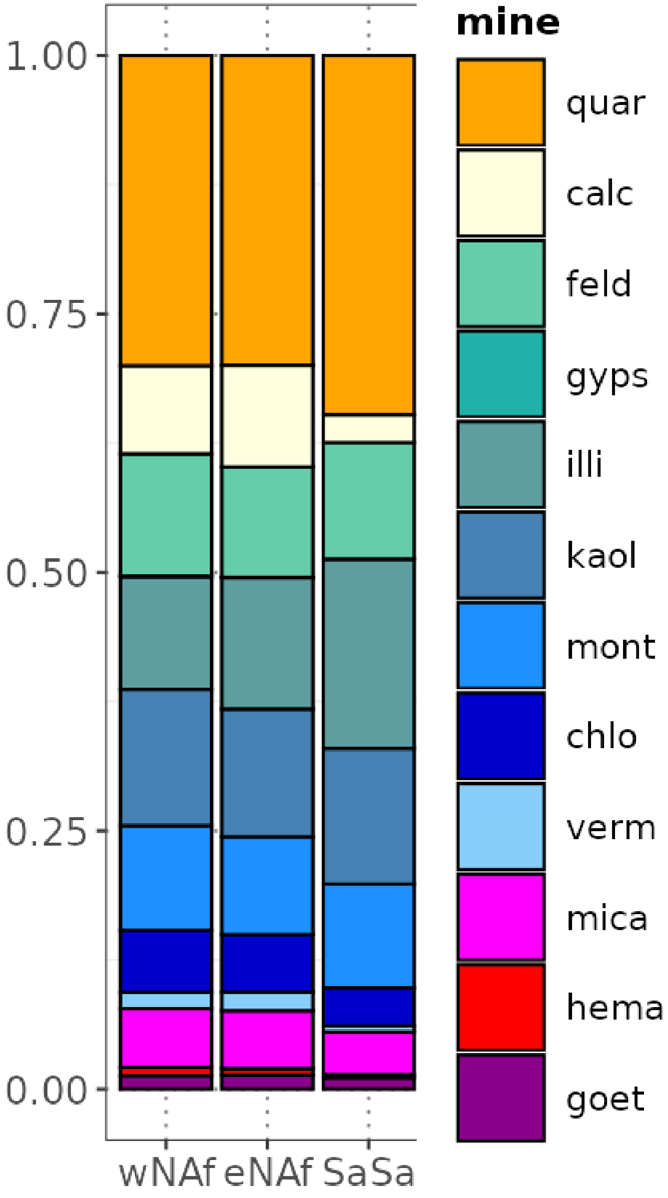
UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH

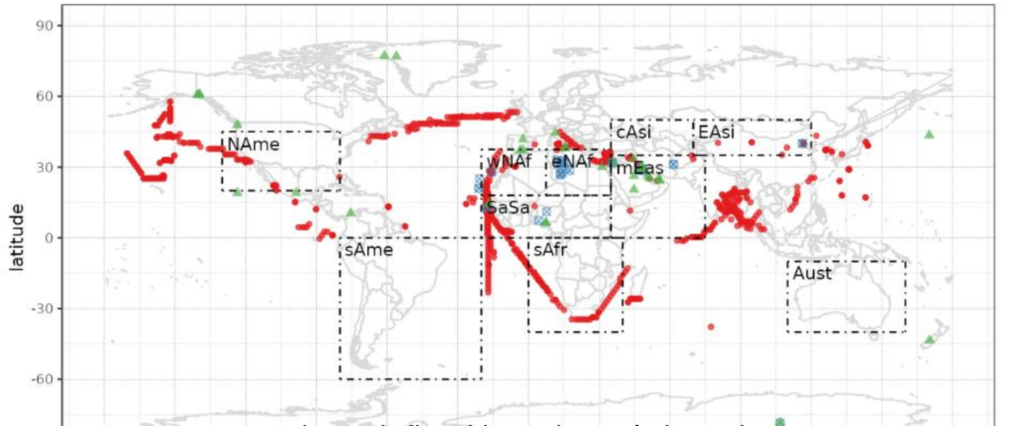
GFDL Seminar
Princeton, 06/06/2023

C1999

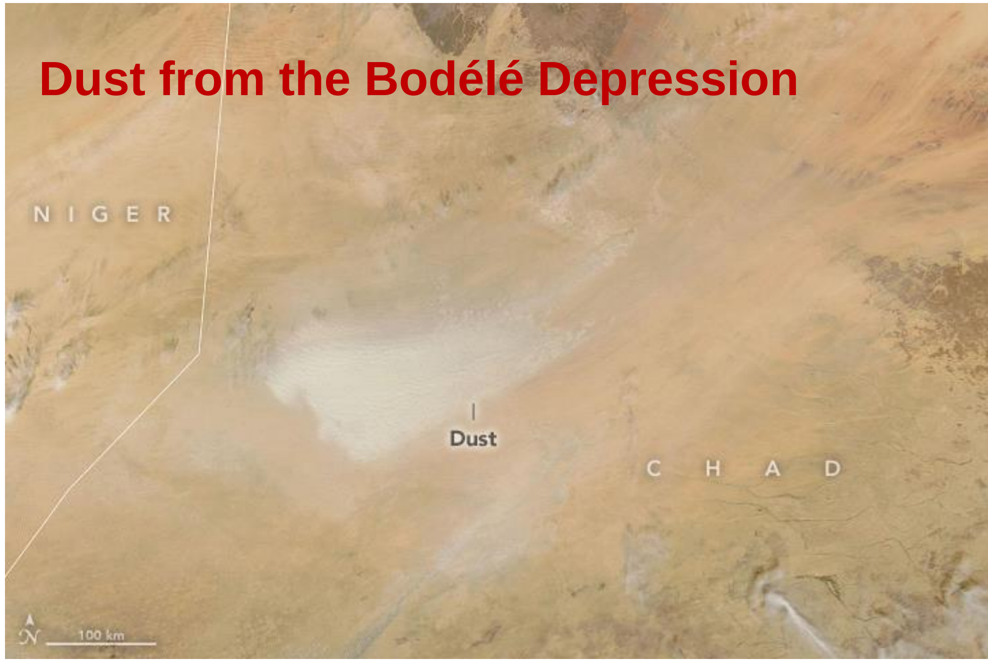


J2014





Dust source regions defined in Kok et al. (2021)



Credit: NASA Earth Observatory images by Lauren Dauphin, using MODIS data from [NASA EOSDIS/LANCE and GIBS/Worldview]

Some models including dust mineralogy

Model	CESM-CAM6	MONARCH	GFDL-AM4	GISS-ModelE	IFS-Aer
Soil mineralogy	C1999	C1999 J2014	C1999	C1999	J2014
PSD	Modal model 3 modes	Sectional model 8 bins	Sectional model 5 bins	Sectional model 5 bins	Sectional model 3 bins
Size range (diameter)	10 µm	20 µm	20 µm	32 µm	40 µm
Emission method	BFT	BFT	BFT	Modified BFT	Projected
Mixing state	Internally mixed	Externally mixed Fraction of iron oxides mixed with other minerals	Externally mixed Fraction of iron oxides mixed with other minerals	Externally mixed Fraction of iron oxides mixed with other minerals	Externally mixed
References	Scanza et al. (2015), Hamilton et al. (2019), Li et al. (2021)	Gonçalves Ageitos et al. (in review), Klose et al. (2021)	Horowitz et al. (2020)	Obiso et al. (2023, in review), Perlwitz et al. (2015a,b)	Remy et al. (2022)

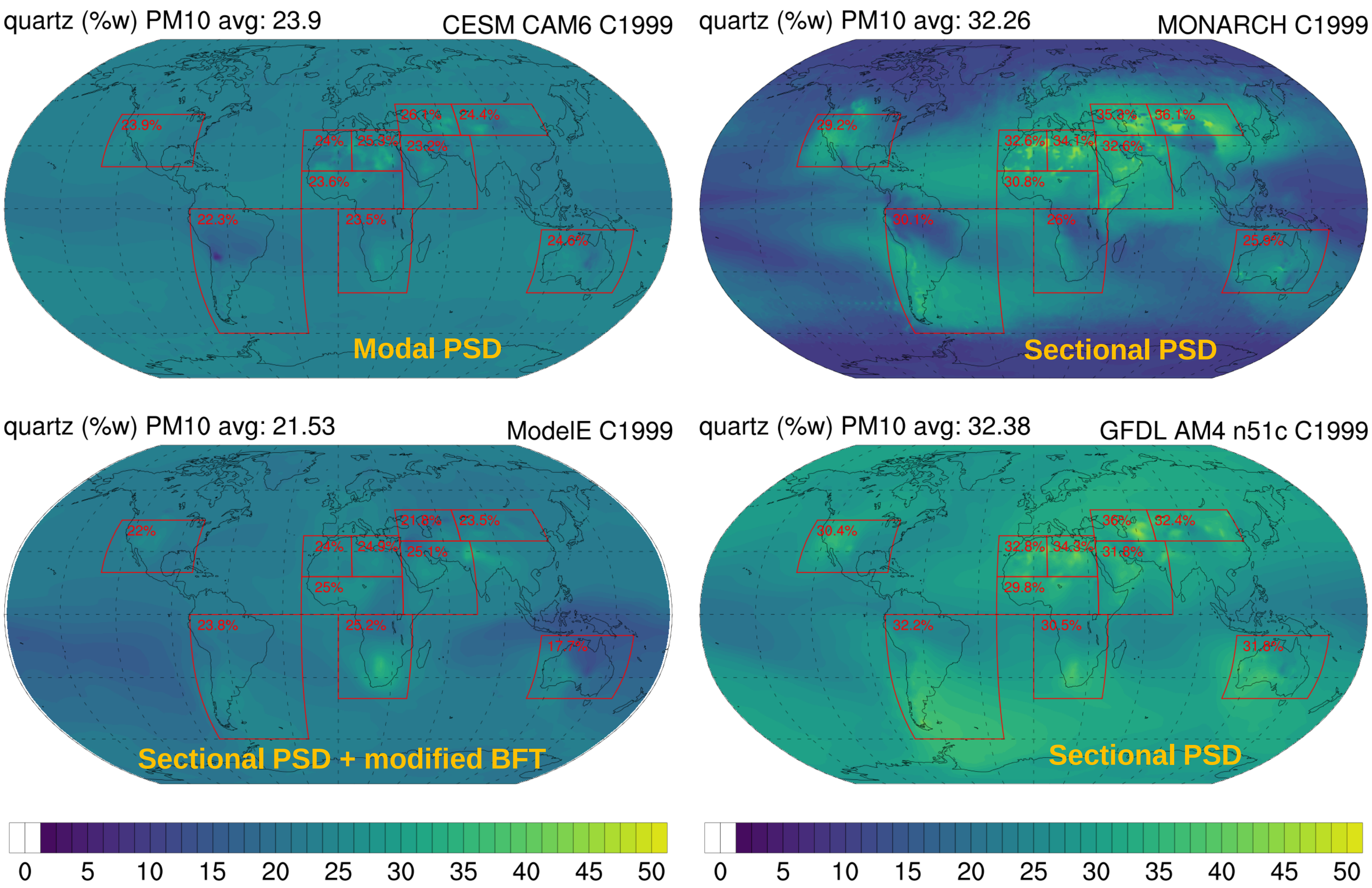
Some models including dust mineralogy

Model	CESM-CAM6	MONARCH	GFDL-AM4	GISS-ModelE	IFS-Aer
Resolution	1º x 1.25º	1º x 1.4º	1º x 1.25º	2º x 2.5º	T255L91 (0.7º)
Simulation period	2007-2011	2006-2010	2001-2020	2011-2020	2017-2020
Mode	Nudged towards reanalysis	Re-initialized every 24 h with reanalysis	Nudged towards reanalysis	Nudged towards reanalysis	Re-initialized with reanalysis

Model data has been provided by L. Li, N. M. Mahowald, Q. Song, P. Ginoux, V. Obiso, R.L. Miller, and S. Remy
In the context of EMIT and CAMS2-35 projects

Variability across models: same soil map.

Quartz mass fraction (%w) at surface PM10 concentration.

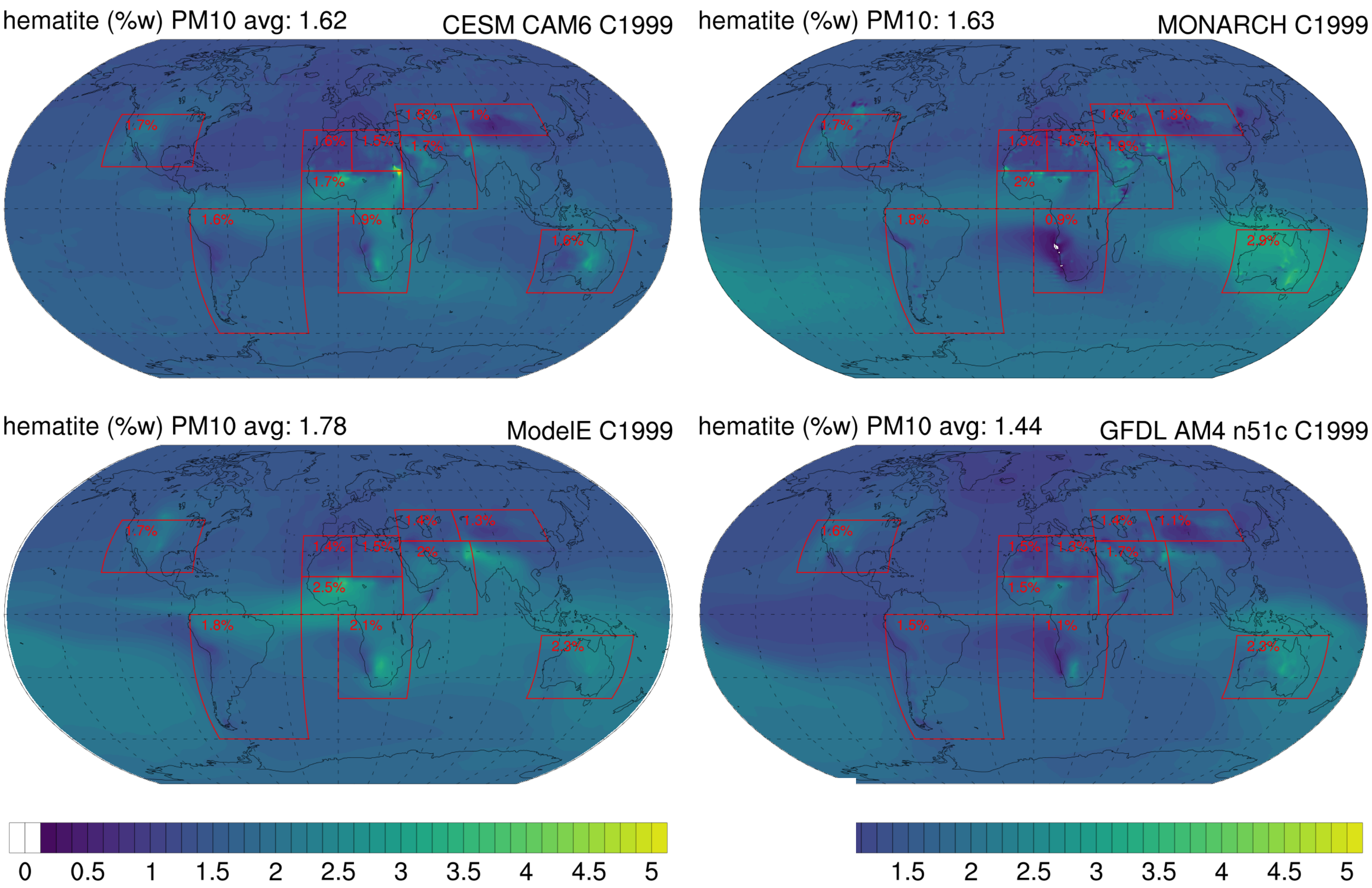


Larger differences in transport or remote regions than over sources.

Differences in the representation of PSD, transport or removal processes → variability across models.

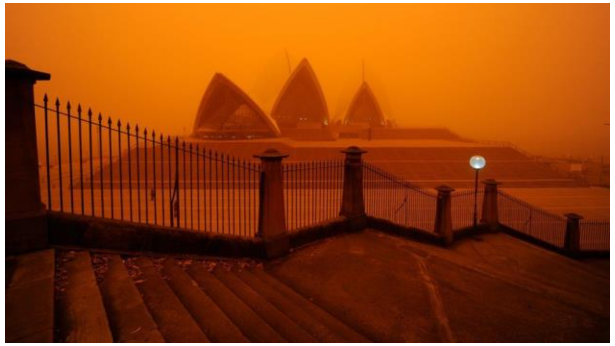
Variability across models: same soil map.

Hematite mass fraction (%w) at surface PM10 concentration.



Common regional differences: contrast Sahara – Sahel

Australia – rich in iron oxides

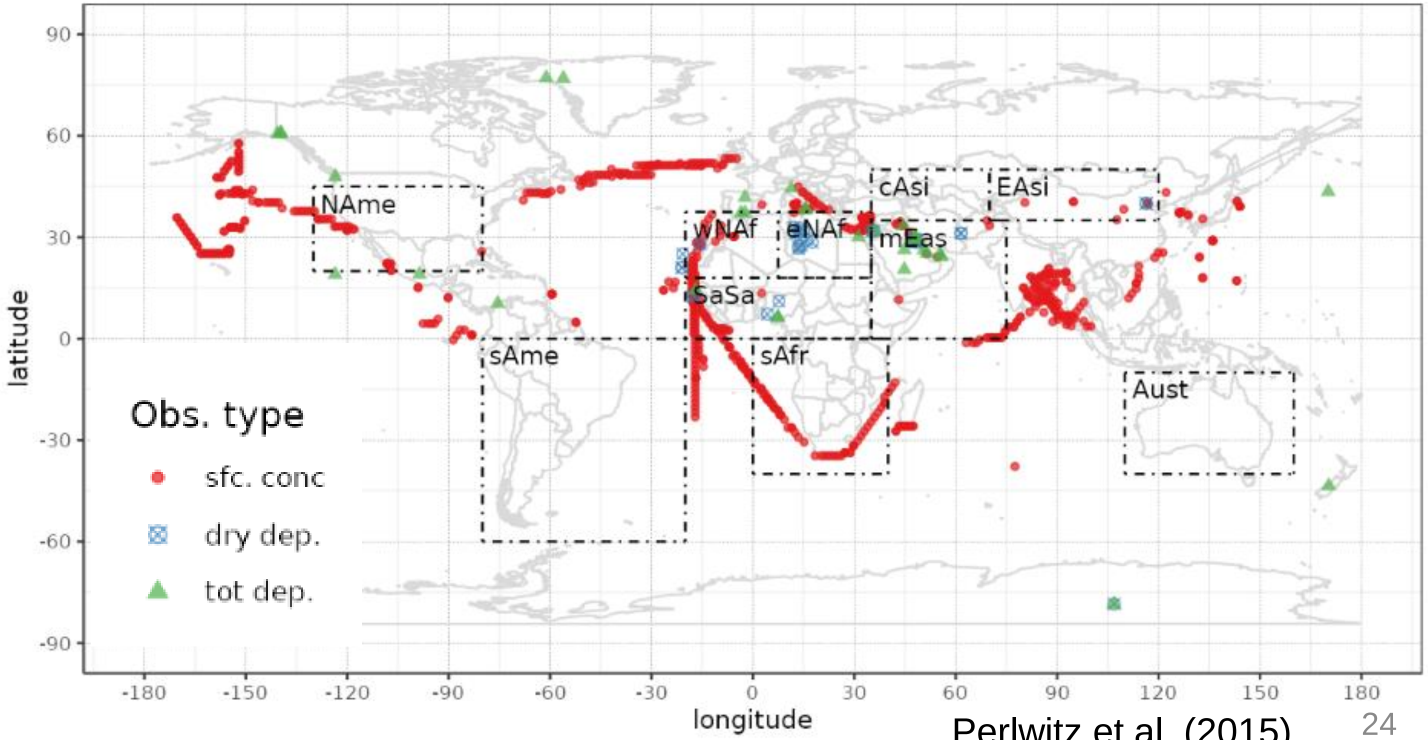


Credit: Getty images

Observations of mineral mass fractions

- Obs. from the late 60’s to date.
- Sampling time vs. model average: Temporal collocation – monthly basis
- Reported minerals vs. modelled minerals: Mineral fractions estimated over those minerals observed AND modelled
- Size range of observations vs. modelled size range: Size collocation

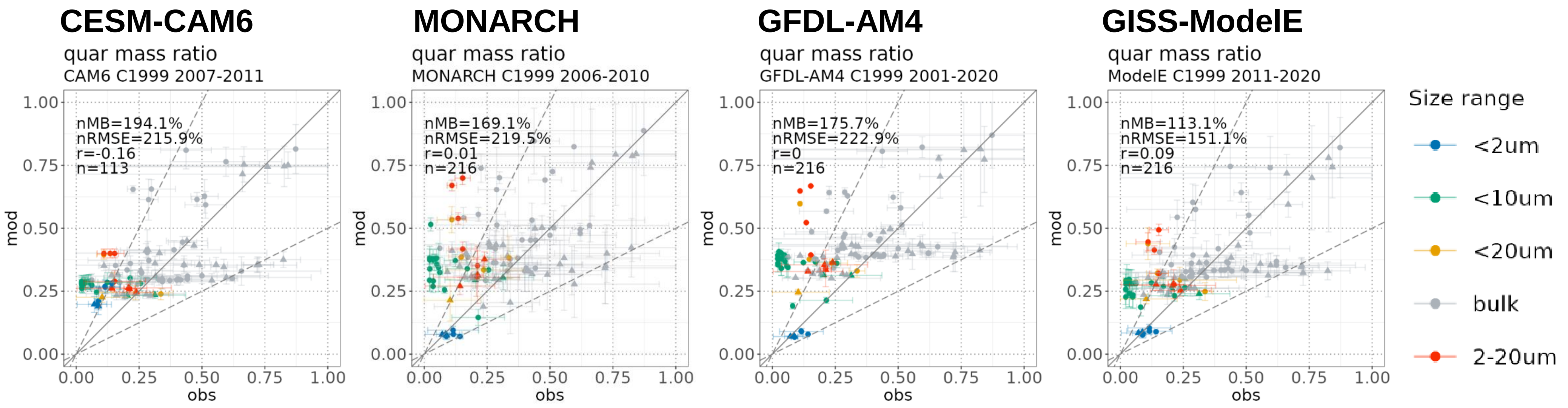
- Statistics in the plots use data in the modelled size ranges.
- Normalized Mean Bias (nMB)
- Normalized Root Mean Square Error (nRMSE)
- Correlation (r)
- Number of measurements in the samples used for the comparison (n)

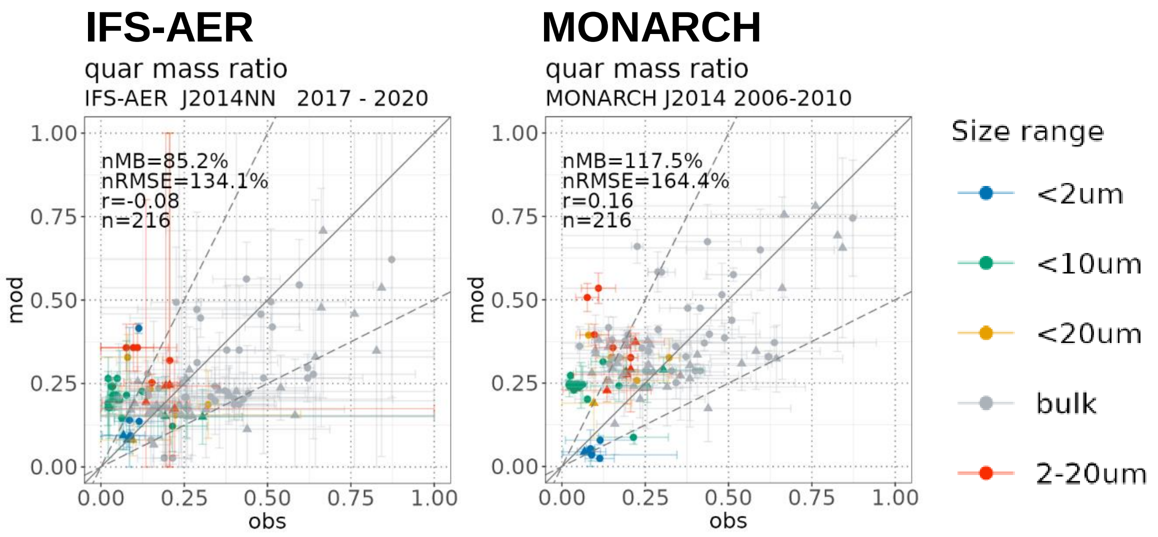


Perlwitz et al. (2015)

Barcelona Supercomputing Center
Centro Nacional de Supercomputación
UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH

Quartz mass fraction evaluation

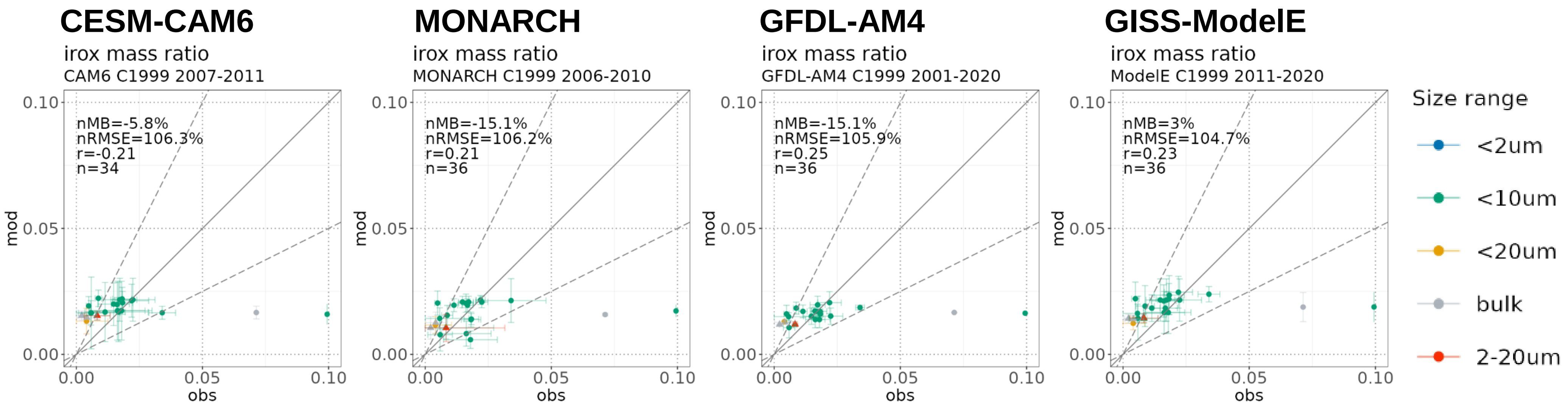


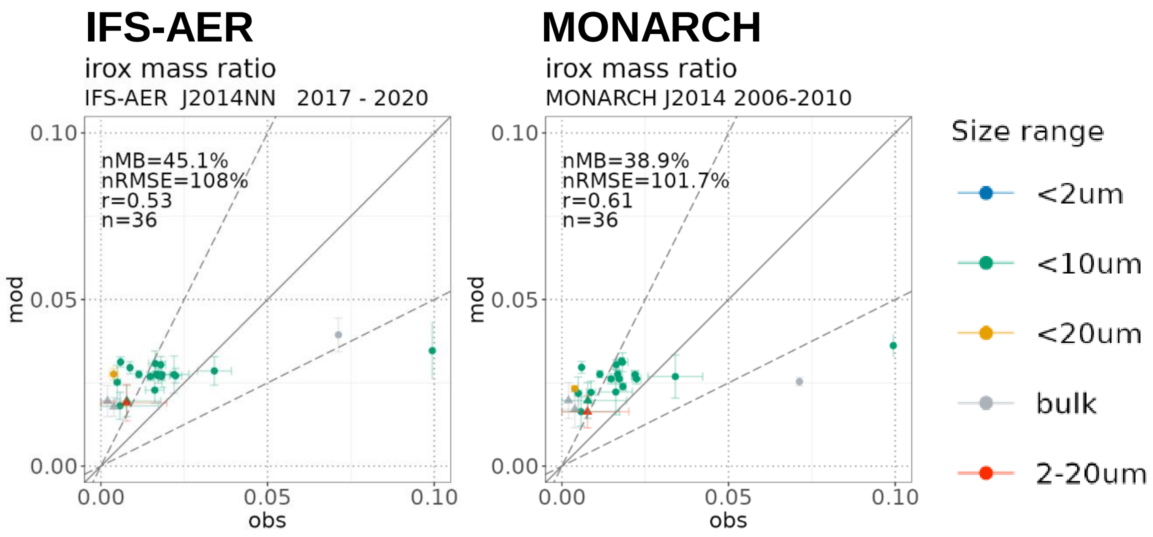


Overestimation of the mass fraction above 2 µm of diameter across models.

Some models also show an underestimation in clay sized fractions (below 2 µm of diameter).

Iron oxides mass fraction evaluation





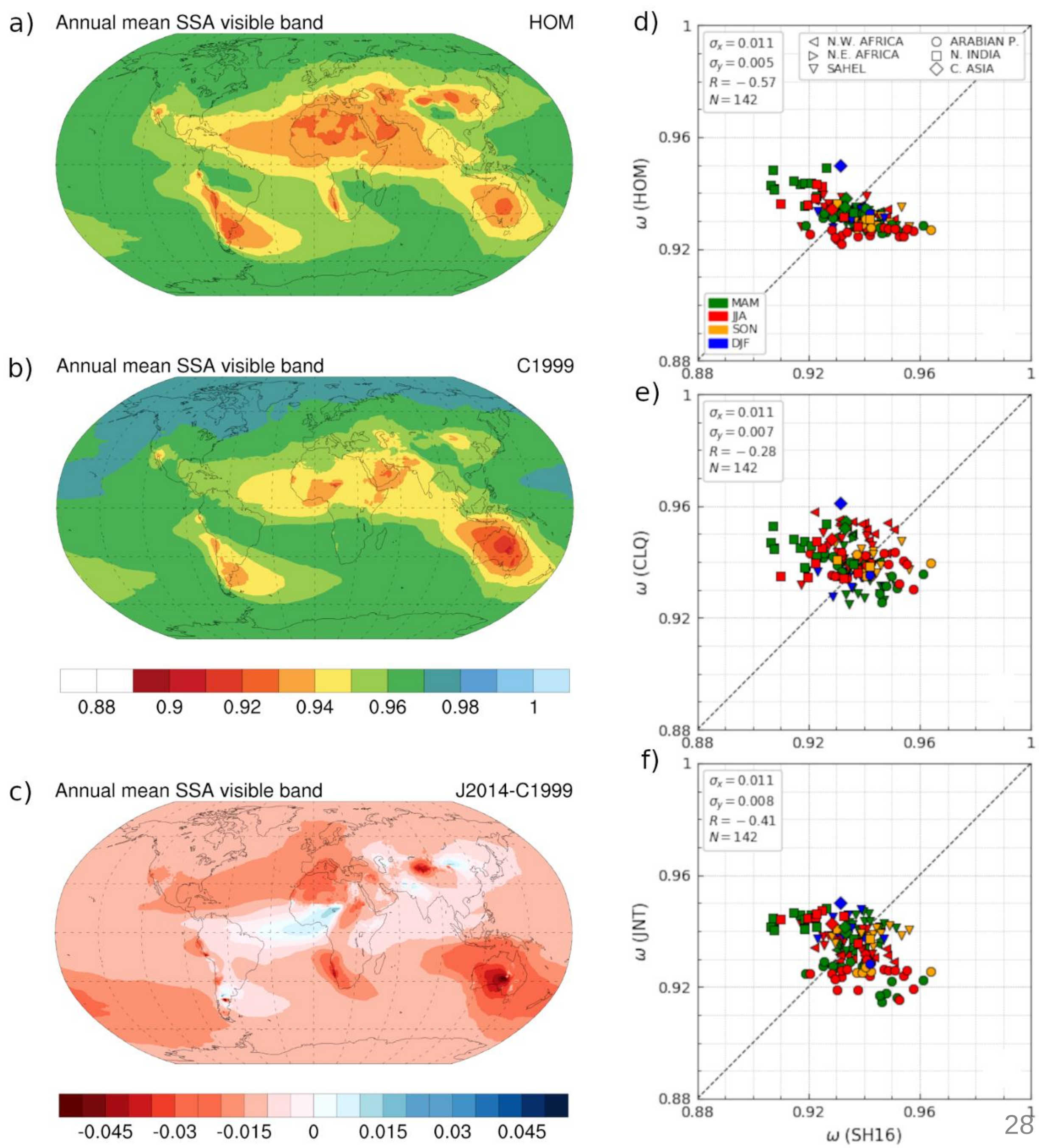
Underestimation in models using C1999 and overestimation in models using J2014.

Potentially, improved spatio-temporal distribution of iron oxides in models that use the J2014 soil map.

Impacts on the climate system

Impact on dust absorption

- SSA in the visible band as derived from MONARCH considering: optically homogeneous dust, C1999 mineralogy and differences when considering J2014.
- *Evaluation against AERONET retrievals filtered following the criteria in Schuster et al. (2016).*



Diagnostics provided by Vincenzo Obiso (NASA-GISS).

Gonçalves Ageitos et al. (2023, in review)

Check also: Obiso et al. (in review, EGUSPHERE:2023-1166)

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

UNIVERSITAT POLITÈCNICA DE CATALUNYA BARCELONATECH

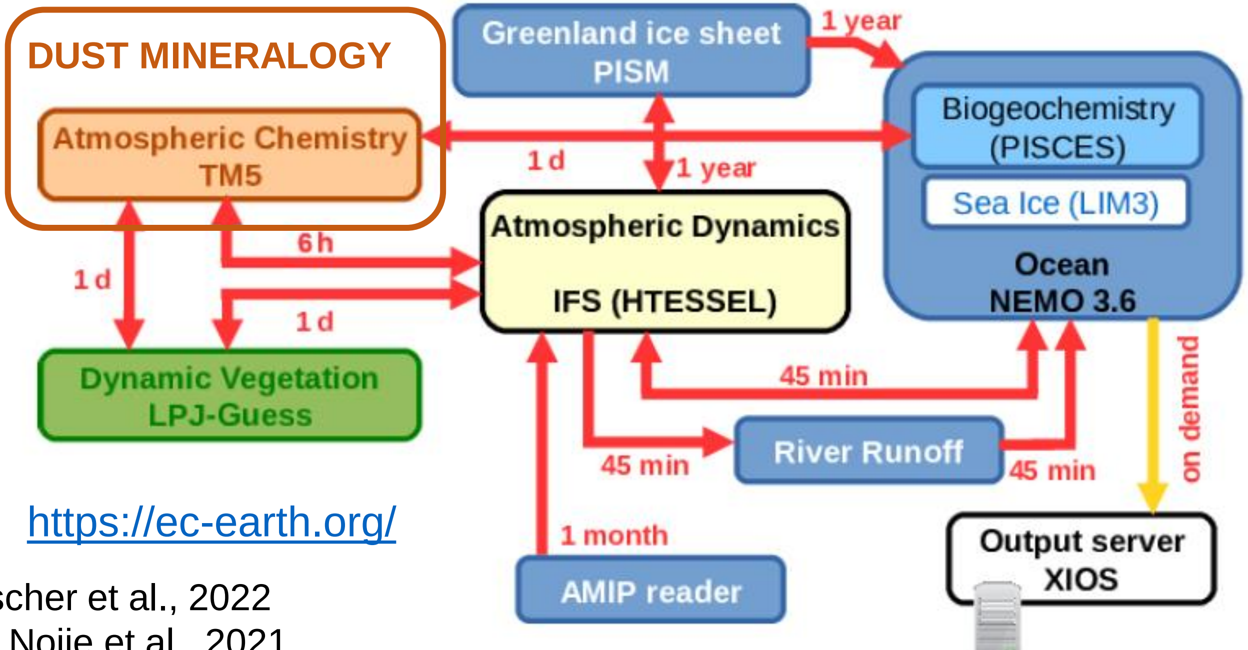
Minimal representation of dust mineralogy in an ESM

TWO SOIL MINERALOGY MAPS: C1999, J2014

BFT to DEFINE MINERALS' EMITTED PSD: Accumulation and coarse modes.

REPRESENTATION OF THE MINERALOGY TARGETING CLIMATE IMPACTS:

- **Calcite** → to explicitly calculate *aerosols' pH* with the ISORROPIAII thermodynamic equilibrium model.
- **Quartz, feldspar** → to estimate *ice nucleating particles.*
- **Hematite, goethite** → to define *dust optical properties* in the SW.
- All minerals → to derive ***iron*** from dust.



https://ec-earth.org/

Döscher et al., 2022
van Noije et al., 2021
Myriokefalitakis et al., 2022

https://ec-earth.org/

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH

Aerosol-sensitive INP parameterizations in EC-Earth3

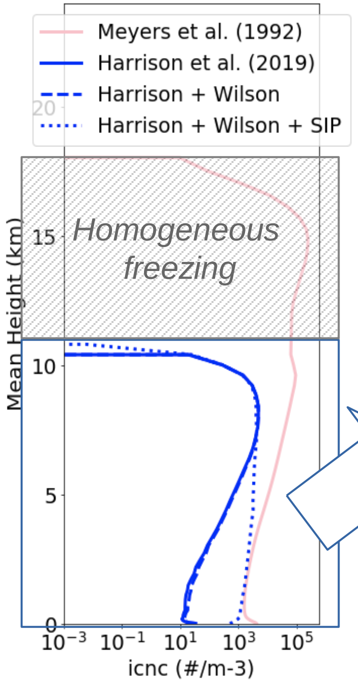
Costa-Surós et al., in prep.

Meyers et al. (1992) – Temperature dependent

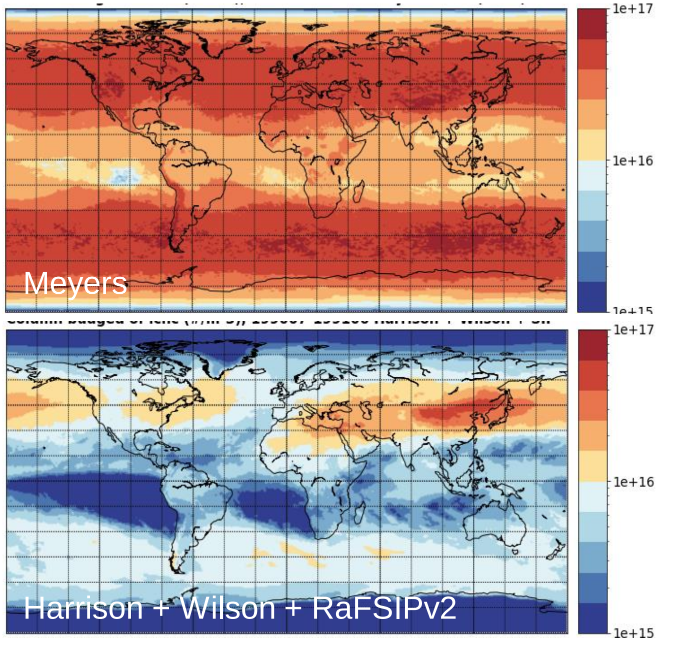
Harrison et al. (2019) – k-feldspar and quartz
Wilson et al. (2015) – marine organic aerosols
Secondary ice parameterization (RAFSIP) - *Georgakaki et al. (in prep.)*

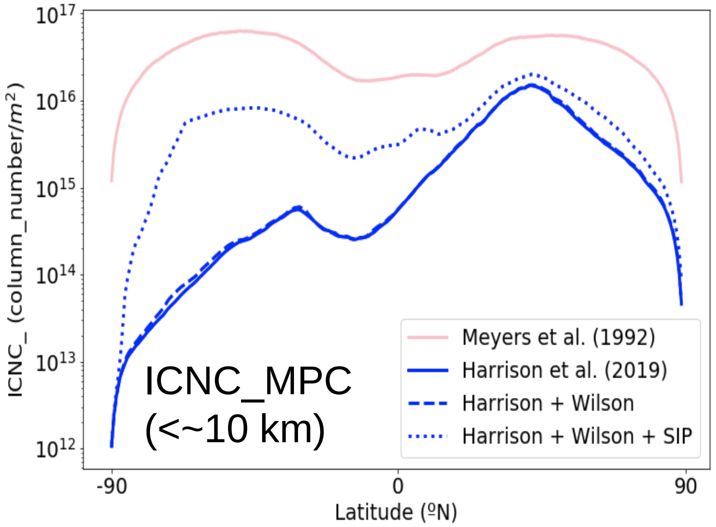
On-going simulations and analyses to determine climate impacts

ICNC_MPC



ICNC_MPC (column burden <~10 km) #/m^3



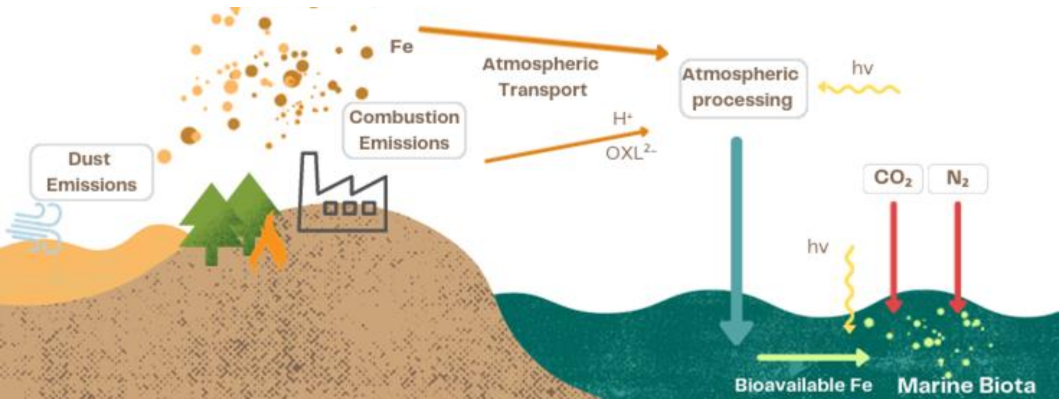


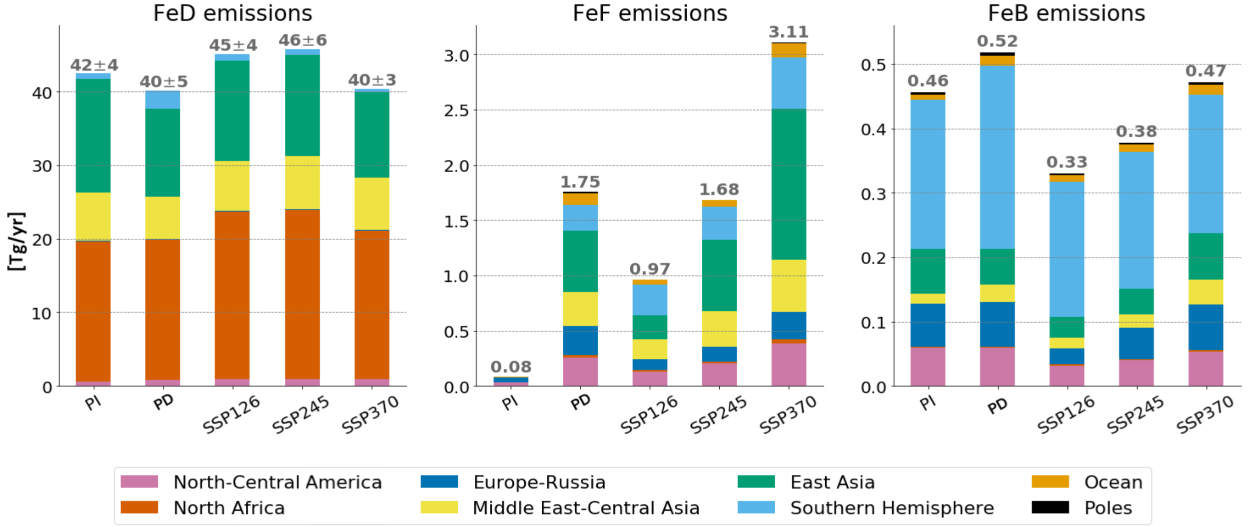
EC-Earth3 FORCeS 1-year nudged experiments with observed sea ice concentration and sea surface temperature

Mineralogy in EC-Earth3-Iron: aerosol pH and soluble iron deposition

Myriokefalitakis et al., 2022
Bergas-Massó et al., 2023

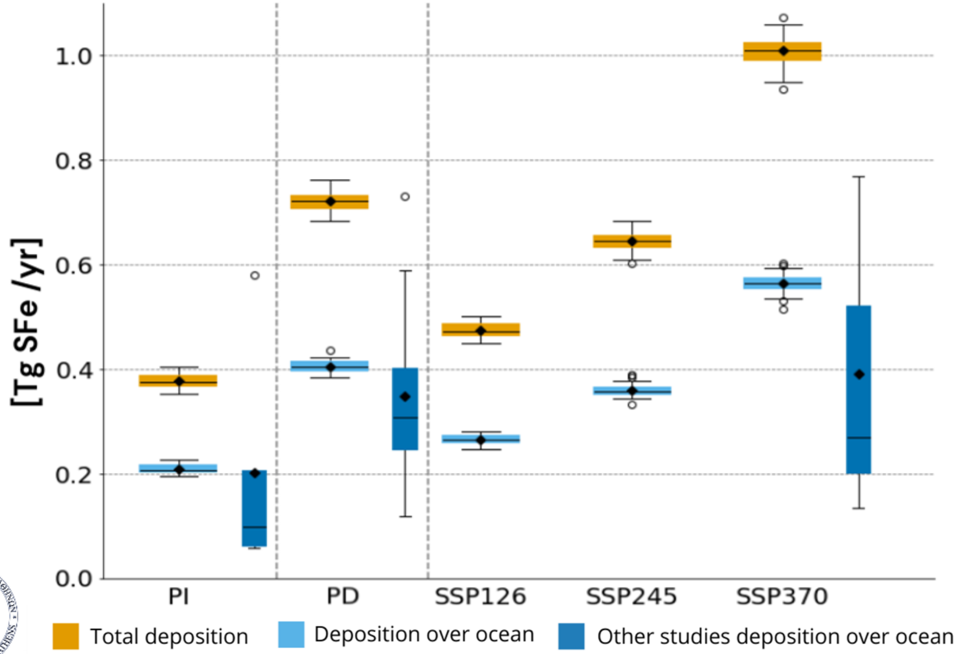
EC-EARTH3-Iron





Mineralogy impacts iron from dust and dissolution rates through its effect on aerosols' acidity.

Increased soluble iron deposition in future scenarios attributed to the increase of dissolution precursors and anthropogenic emissions



Barcelona Supercomputing Center
Centro Nacional de Supercomputación

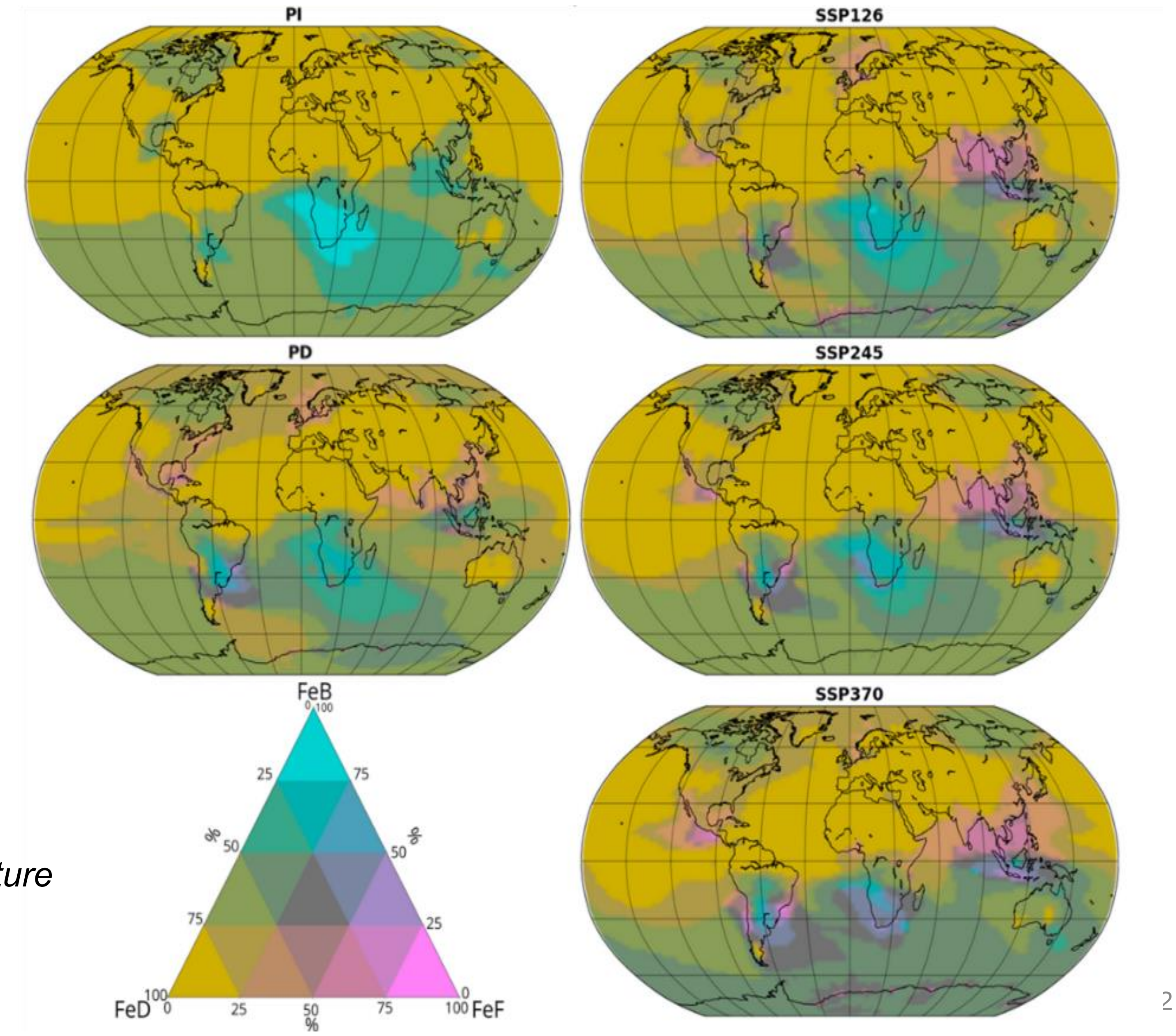
UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH

DOMOS

Royal Netherlands Meteorological Institute
Ministry of Infrastructure and Water Management

Source contribution to soluble iron deposition

Relative contribution of **biomass burning**, **anthropogenic combustion** and **mineral dust** sources to the soluble iron deposition in past, present and future climate scenarios.



Bergas-Massó et al., 2023
Recently published in Earth's Future

Open questions and future research

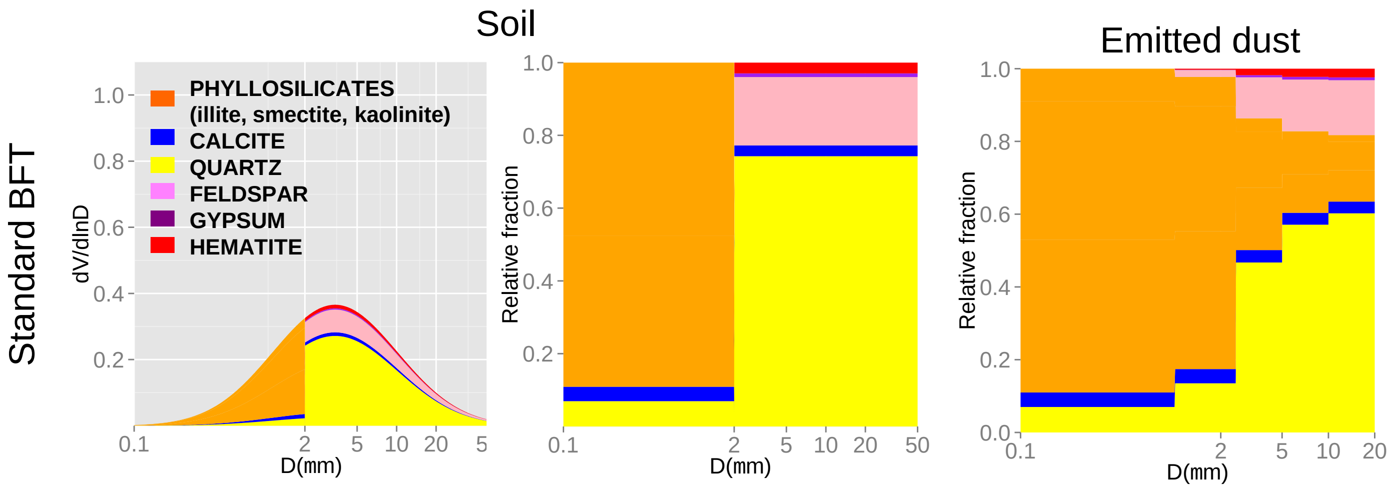
On-going and future work

- Impact of **mineral-dependent** dust **optical properties** and **INP** in **long-term climate** experiments (e.g., FORCeS and AEROCOM DURF experiments) with EC-Earth3.
- Assess the contribution of **anthropogenic dust sources** and **improved biomass burning** emissions upon **soluble iron** deposition with EC-Earth3-Iron.
- Exploit FRAGMENT ERC (experimental campaigns in Morocco, Iceland, US and Jordan) data to further **constrain the minerals emitted size distribution**.

Summary and conclusions

- Common soil map and emission method → Variability across models due to different size distribution, transport and removal processes.
- Similar evaluation metrics against mineral fractions (likely dominated by observations close to sources)
- Relevance of the size-distributed mineralogy at emission (e.g., overestimation of quartz in aerosol silt sizes).
- Issues with the soil maps, particularly relevant for iron oxides
- Significant impact in our model results: dust SSA, ice crystal number concentrations, iron emission and dissolution.

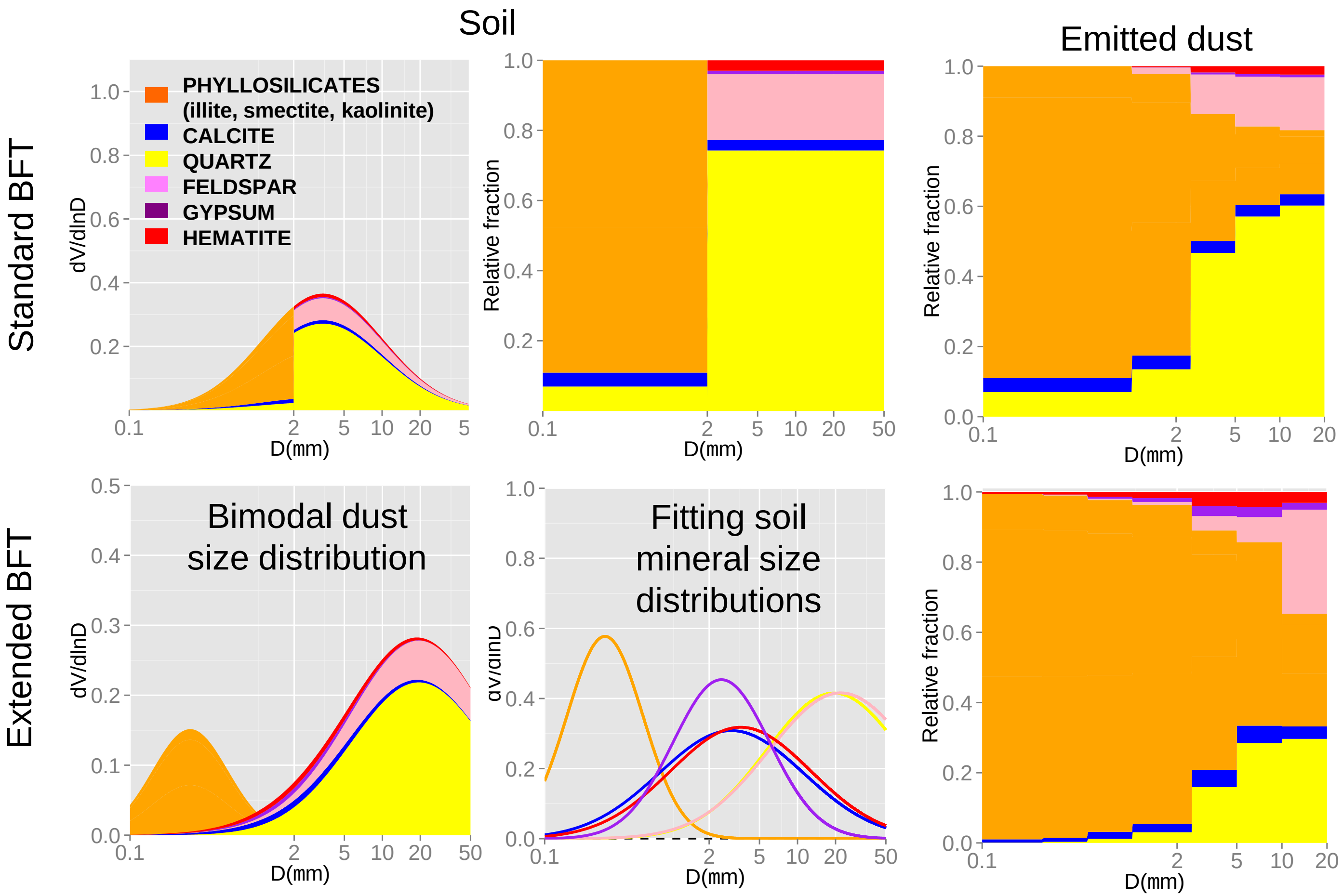
Refining the mineral fractions at emission



Perlwitz et al., 2015a,b; Pérez García-Pando et al., 2016;

Extended BFT proposed by C. Pérez García-Pando

Refining the mineral fractions at emission



Perlwitz et al., 2015a,b; Pérez García-Pando et al., 2016;

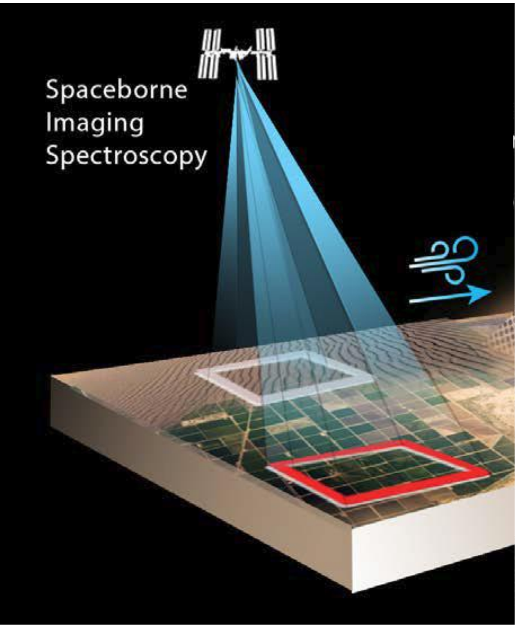
Pérez García-Pando et al., in prep.

Extended BFT proposed by C. Pérez García-Pando

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

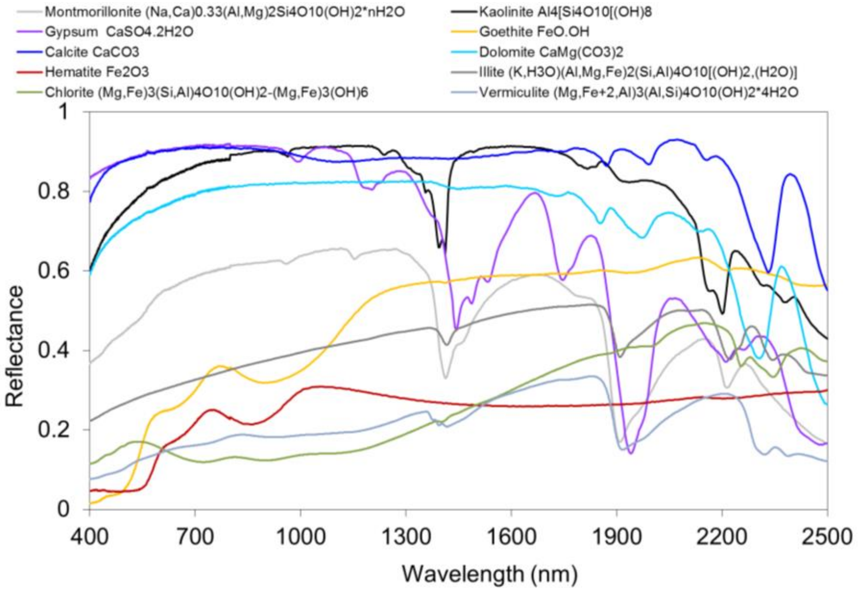
UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH

New mineralogy maps from NASA EMIT (Green et al. 2020)

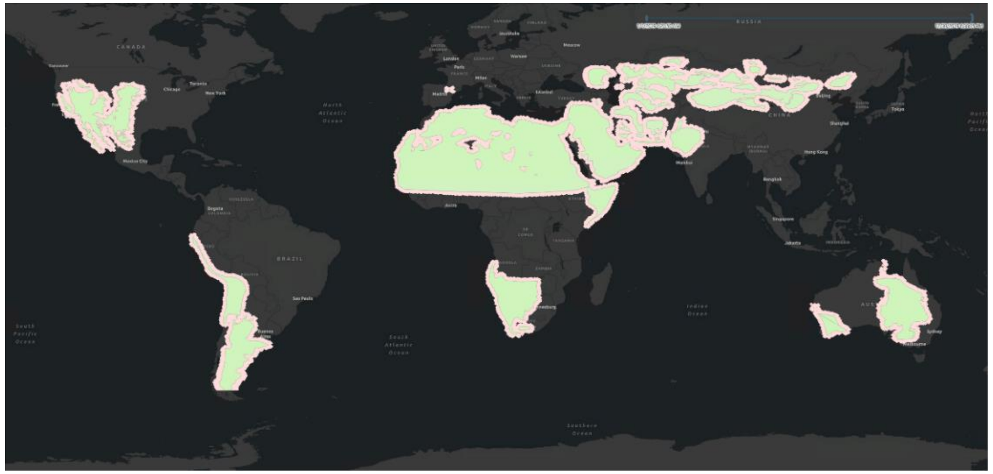


The EMIT instrument is measuring from the ISS since July 14, 2022.

VSWIR Spectra of Dust Source Minerals



Dust Minerals have distinct spectral signatures



Target mask for EMIT retrievals covering arid land regions

Level 3 products – map of 10 (+2) minerals to be used within ESMs

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

UNIVERSITAT POLITÈCNICA DE CATALUNYA BARCELONATECH

Jet Propulsion Laboratory
California Institute of Technology

EMIT

Thank you !

Acknowledgments

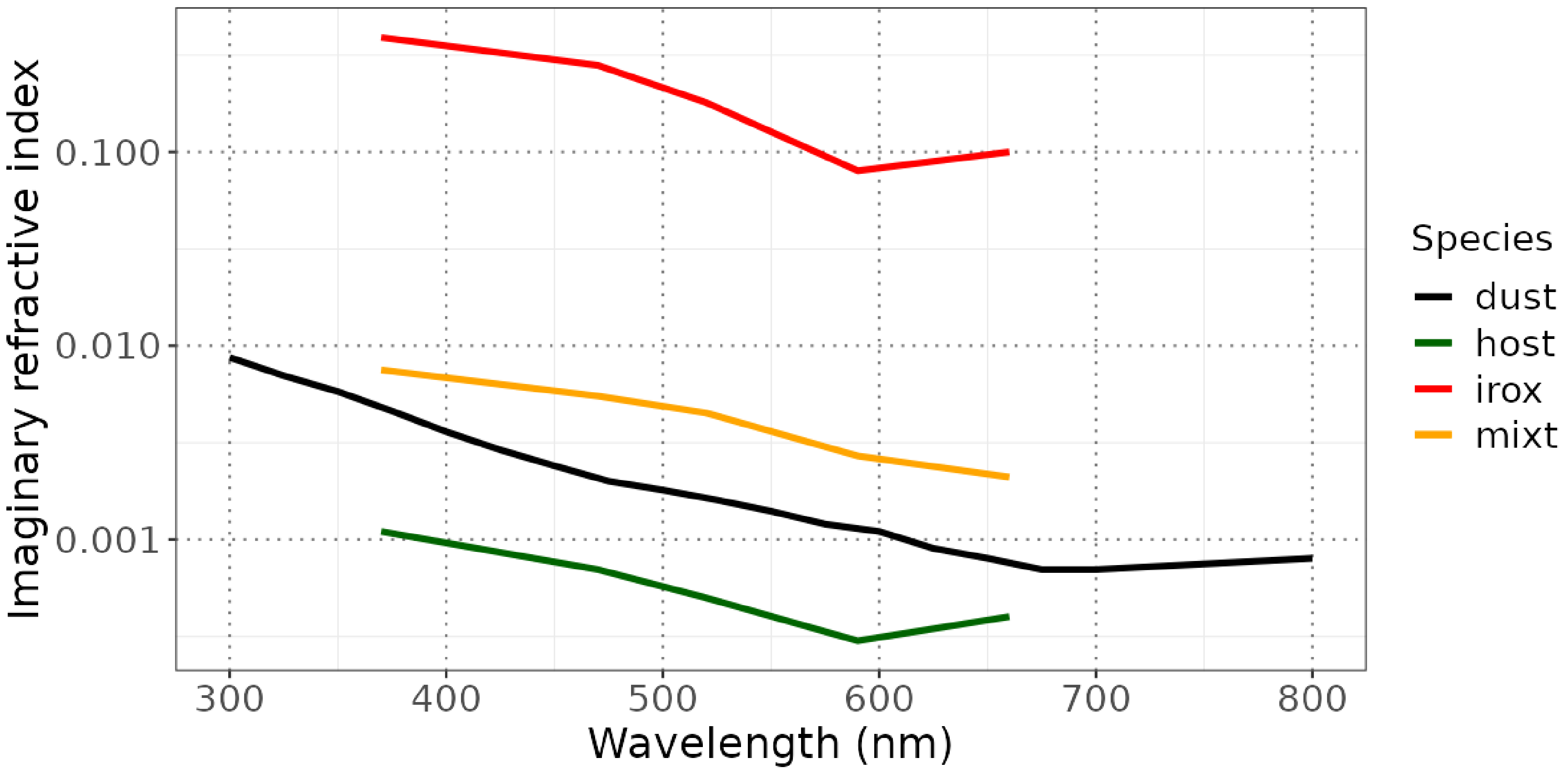
Carlos Pérez García Pando
Oriol Jorba
Elisa Bergas
Montse Costa
and many more collaborators from BSC

Qianqian Song (NOAA-GFDL)
Paul Ginoux (NOAA-GFDL)
Vincenzo Obiso (NASA-GISS)
Ron Miller (NASA-GISS)
Longlei Li (Cornell U.)
Natalie M. Mahowald (Cornell U.)
The EMIT team

Stelios Myriokefalitakis (NOA)
Marios Chatziparaschos (U. Crete)
Maria Kanakidou (U. Crete)
Anasthasios Nenes (EPFL)
Georgakaki Paraskevi (EPFL)
Twan Van Noije (KNMI)
Philippe Le Sager (KNMI)

- This work was supported by the ERC Consolidator Grant FRAGMENT (grant agreement No. 773051), and the AXA Chair on Sand and Dust Storms at BSC funded by the AXA Research Fund both led by Dr. Carlos Pérez García Pando.
- The research leading to these results has also received funding from the Spanish Ministerio de Economía y Competitividad as part of the NUTRIENT project (CGL2017-88911-R), the H2020 GA 821205 project FORCeS, and the ESA-DOMOS project.
- We thankfully acknowledge the computer resources at Marenostrum4, granted through the PRACE project eFRAGMENT2 and the RES project AECT-2020-3-0020; the technical support provided by the BSC, and the work of all the members of the BSC Earth Science Department group who contribute to the MONARCH model and infrastructure developments.
- Thanks to all the providers of the observational data used for the model evaluation.

Dust and mineral refractive indexes MONARCH



- Host minerals: refractive index from Scanza et al. (2015) with abundances as median of DiBiagio et al. (2019)
- Accretions: assumed 5w% of hematite, RI interpolated from DiBiagio et al. (2019).
- Pure iron oxides: fitting DiBiaggio et al. (2019) with MG mixing rule.

- Homogeneous dust refractive index from Sinyuk et al. 2003.

New heterogeneous ice nucleation parameterization

ICNC estimation

Temperature-sensitive ice nucleation parameterization

Meyers et al. (1992): deposition-condensation freezing

$$N_i = 1000exp[12.96(e_{sl} - e_{si})/e_{si} - 0.639]$$

N_i: ice crystal number concentration
e_{sl}: saturation vapor pressure with respect to liquid water
e_{si}: saturation vapor pressure with respect to ice

Aerosol-sensitive ice nucleation parameterization

PRIMARY ICE PRODUCTION

Immersion freezing

Atkinson et al. (2013): K-fedlspar
or
Ullrich et al. (2017): soot and dust
or
Harrison et al. (2019): K-feldspar and quartz

+ **Wilson et al. (2015)**: of marine organic aerosols

SECONDARY ICE PROCESSES

Georgakaki et al. (in prep.): RaFSIP, which considers:
- Hallet-Mossop process
- Droplet shattering during freezing
- Fragmentation due to collisional break-up

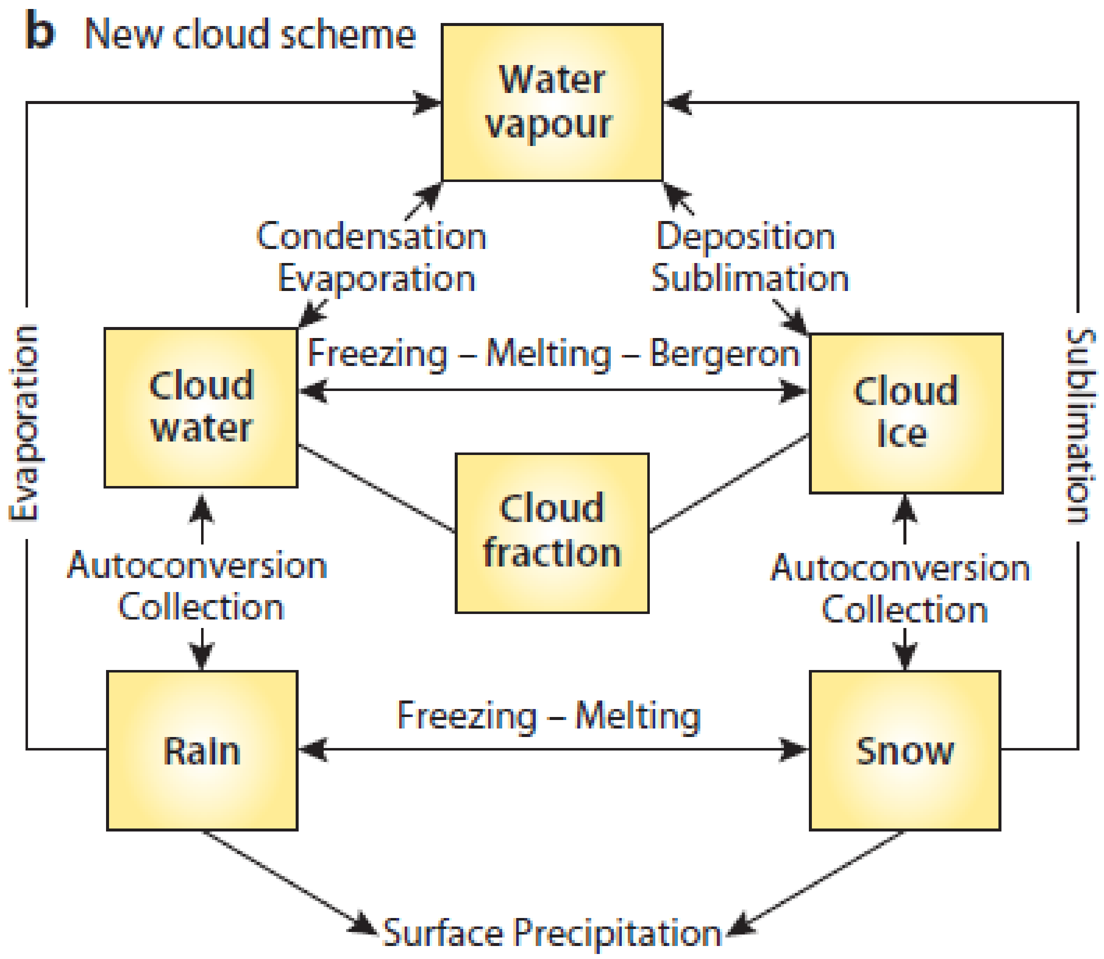
Ice crystal growth by vapor deposition

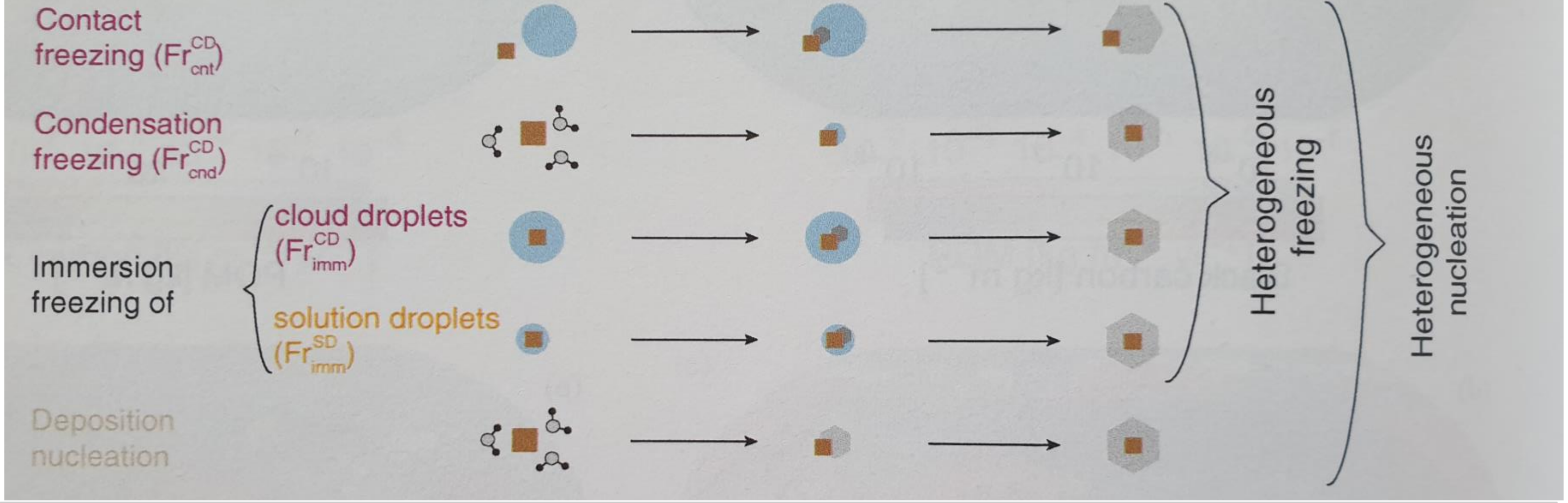
Depositional growth parameterization

Following Pruppacher and Klett (1997) and Rotstayn et al. (2000)

Costa-Surós et al., in prep.

IFS cloud microphysics





Collision fragmentation,
Hallett-Mossop or rime-splintering
Droplet shattering
Sublimation fragmentation

SIP

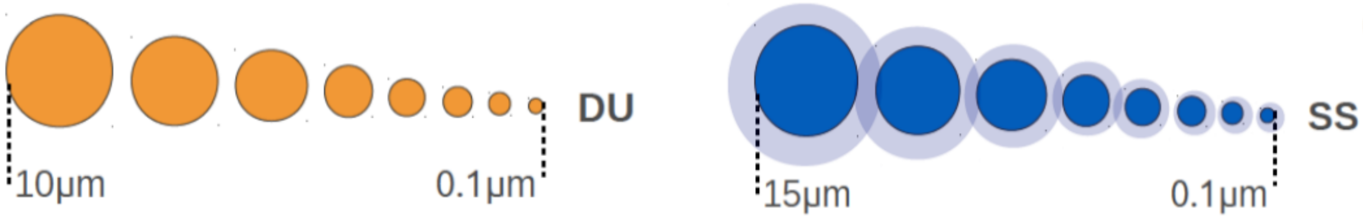
Lohmann et al., 2016

MONARCH

Aerosol Scheme

Sectional

dust (DU)
sea-salt (SS)

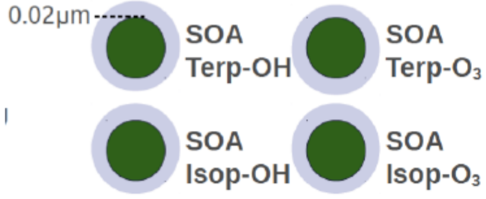


Bulk

Black Carbon (BC)

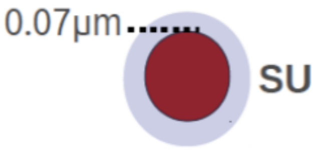
Organic Aerosols (OA)

Primary Organic Aerosols (POA)
Secondary organic aerosols (SOA)
4 gaseous tracers (OH, O3, TERP, ISOP). Online emission (MEGAN)
4 aerosol-phase hydrophilic tracers
2-product scheme of Tsigaridis and Kanakidou (2007)
Oxidation by OH and O3 and gas-particle partitioning
Anthropogenic SOA from Toluene and Xylene under development



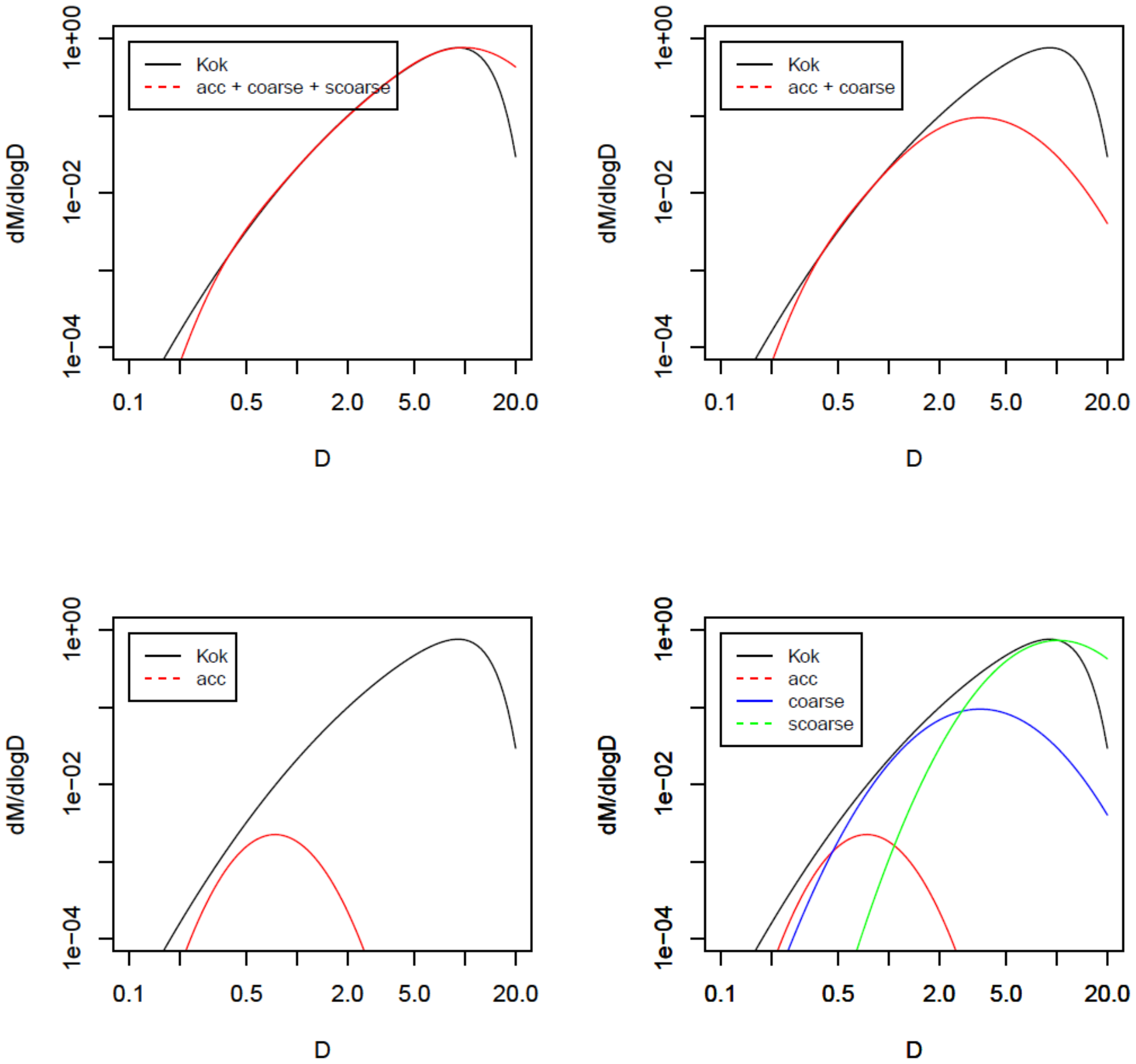
Sulfate (SU):

4 additional prognostic tracers (SO2, DMS, H2O2, H2SO4)
3 online or climatological oxidants (OH, O3, HO2)
gas-phase oxidation of SO2, DMS and H202 by OH
aqueous-phase oxidation by H202 and O3



Nitrate (NO3) and Ammonium (NH4): as calculated by EQSAM thermodynamic equilibrium model but not evaluated yet

Kok size distribution fitted with modal PSD



Thanks to C. Pérez García-Pando